A Dissertation

entitled

**CFD Investigation of Metalworking Fluid Flow and Heat Transfer in Grinding**

by

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Metalworking fluids have an exceptional role in grinding. Correct fluid application results in enhanced process stability, better work piece quality and tool life. This work aims to create and use Computational Fluid Dynamics (CFD) models in order to simulate the fluid flow and heat transfer in a grinding process, as a better alternative to many experiments that are expensive, time-consuming and with very limited ability. The features of created 2-D and 3-D models are described in detail, along with results obtained, and proposals for the future work. The results show very detailed distributions of temperatures, pressures and flow rates in and around the grinding region. By generating a very detailed picture of the grinding process itself, the data obtained is essential in studying the influence of the grinding fluid on the grinding process, as well as in determining the best fluid composition and supply parameters for a given application. The results agree well with experimental global flow rates and temperature values and show the feasibility of both 2-D and 3-D simulations in grinding applications, and performed parametric studies can be an useful tool in optimizing grinding processes.
To my family and friends.
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Chapter One

Introduction

1.1 Grinding and grinding fluid applications

Grinding is one of the most important processes in manufacturing. It is a modern machining process with high-speed abrasive wheels, pads and belts. The main characteristic of grinding is that it results in production of components with:

- High precision (low tolerances)
- High surface finish (low roughness).

Because of this, grinding is mostly used as the final machining process in manufacturing of parts with high requirements. Relative to other machining processes, grinding is expensive and requires a high energy input per volume of material removed. There is a relatively large contact area between the tool and the workpiece and there is high friction between abrasive the grits and the workpiece surface. This leads to difficulties in supplying coolant to the grinding arc, thus resulting in a high risk of thermal damage to the workpiece surface layer as well as loading and wear of the grinding wheel. Thermo-mechanical processes in the contact zone are defined by
tribological relationships between the grain cutting edge, the grinding wheel bonding, the workpiece and the chip as it forms, so that cooling and lubrication play a decisive role during grinding with respect to heat generation and dissipation. Experience has shown that in addition to coolant type, composition and filtration, coolant supply (nozzle position, nozzle geometry, supplied flow rate and jet characteristics) can influence process productivity, workpiece quality and tool wear considerably.

1.2 Motivation and objectives of this work

The objective of this work is to adapt and apply the approach and methods used in computational fluid dynamics (CFD) to determine the role of the metalworking fluid in grinding, and to study the grinding process itself.

In essence, many aspects of the grinding process with a process fluid are well understood and documented, both theoretically and experimentally. On the other hand, grinding is an extremely complex process, in which many dissimilar but interrelated physics have comparable weight; these are topics of material science (such as elastic/plastic deformation, breakage), fluid dynamics (flow under high pressures and temperatures, and solid-liquid interaction), and heat transfer (conduction, convection, phase change), all in the context of a complex and changing geometry with different length scales. Lubricity is a metalworking fluid property that measures its effectiveness in reducing friction. For metalworking fluids, lubricity is a property determined experimentally. The experimental procedures to determine this property vary – many manufacturers use proprietary methodologies. The procedures are not meant to determine
a value for lubricity, but rather to compare fluids between them, and catalog them in the order of their perceived lubricating qualities. It is clear that the experimental procedures, by looking only at the global lubrication effect, are not capable of distinguishing between different mechanisms of lubrication, nor do they explain why some fluids are better than others in a given application. To find an explanation, the fluid manufacturer must rely on their experience and on personal interpretations related to chemical and, to a less extent, physical properties of the different components in the fluid relative to the workpiece and wheel materials. As a consequence, the formulation of a new process fluid can be associated to a form of art. Gaining knowledge through computer simulations on how changes of each fluid property will be reflected in changes of the grinding process itself, the formulation of a better, or optimum, process fluid for a given application will become possible.

There have not been many numerical investigations of fluid flow and heat transfer in grinding process, and no multiphase flow simulation has been found in the available literature. Previous CFD works in this field concentrated on metalworking fluid single-phase flow inside the delivery system/nozzle and single phase boundary-layer air flow around the grinding wheel and scrapers.

CFD analysis of grinding systems has a significant potential to provide valuable insight to what is physically happening to metalworking fluid, grinding wheel and workpiece and how does the fluid itself influence the whole grinding process. Analyzing various patterns, such as velocity, fluid path, fluid volume fraction, heat transfer and temperature fields in the fluid and solids helps identify the most important and critical areas within the grinding system and grinding process that require design optimization.
CFD methods and analysis are cost effective alternative to trial-and-error experimental testing, which not only require significant energy and financial resources but also prolong the development phase.

The most modern advances in grinding technology could not be possible without being accompanied by parallel developments in the area of fluid application. Despite the known successes there remains a very significant potential to accelerate the improvements by better understanding of grinding fluid flow, heat transfer and system design. CFD investigations can lead to a wealth of information that can provide valuable insights to designers for grinding process and equipment optimization and more efficient delivery of grinding fluid.

1.3 Grinding fluid functions and types

Coolants play a very important role in machining. Correct fluid application normally results in enhanced process stability, better workpiece quality and tool life. A grinding fluid serves a number of purposes:

- Lubrication
- Cooling in the contact area
- Bulk cooling outside the contact area
- Flushing of the debris away from the contact area
- Entrapment of abrasive dust and harmful vapors
The main purpose of grinding fluids is to reduce grinding temperatures. This is obtained in two different ways. The first is by directly cooling the process within the grinding contact area. The second is by maintaining wheel cutting efficiency. An important way of reducing temperature is by lubrication, i.e. reducing friction and wear of the grinding wheel, thus minimizing specific energy. In shallow-cut grinding, lubrication is often more significant than direct cooling [1].

Lubrication is very important for reducing wheel dulling. This is achieved by reduction of the friction that develops in the contact zone between tool and workpiece as well as between tool and chip. By decreasing friction and wheel dulling, consumed power is reduced so that less heat is generated and temperatures are reduced. This can greatly improve quality of grinding process and allow higher removal rates [2].

An abundant amount of coolant on and around the workpiece assists bulk cooling, which is, by definition, cooling that takes place outside the contact area [1]. If the workpiece bulk temperature and coolant temperature are allowed to increase, control of the grinding process and outcome will be poor and there is increased risk of thermal damage since any rise in the local temperature in the contact area contributes to the rise in the bulk temperature [2].

Fluid supply helps by flushing chip away from the grinding zone. This is considered essential to avoid recirculation of chip and fractured grain particles which can damage both wheel and the workpiece surface. Recirculated debris damage the wheel surface by adhering to the wheel resulting in deep scratching in the workpiece surface [1].
The combination of lubrication and cooling effects reduces dulling of the grinding wheel and enhances quality of the surface and dimensional accuracy of the workpiece. Cooling and lubrication requirements are different for every application and mostly depend on grinding conditions. Coolants should, ideally, be composed to go well with each specific case. Coolants consist of a basic fluid, to which are added other products such as anti-wear, anticorrosion or emulsifying agents, called additives.

The basic physical properties of all grinding fluids are:

- Density
- Kinematic viscosity
- Surface tension
- Specific heat capacity
- Thermal conductivity
- Heat of evaporation
- Boiling temperature

A good grinding fluid should have:

- High specific heat capacity, $c \text{ [J/(kg*K)]}$
- High thermal conductivity, $k \text{ [W/(m*°C)]}$
- Low viscosity (to be brought easily into grinding area and using low power for pumps)
- Good adhering capability to surfaces which need cooling and lubrication.
If possible, manufacturing engineers reduce the number of grinding fluids used in the production to simplify the problem of purchase, storage and disposal. This approach can considerably reduce operating costs. Therefore, compromises have to be made between optimum grinding performance and flexibility of application of a fluid to a number of processes.

One of the most widely used classifications of metalworking fluids is [24]:

- Oil based coolants:
  - Basic oils (with or without additives): mineral oils, hydrocracked oils, polyalphaolefines, synthetic esters
- Water based coolants:
  - Coolant emulsions (concentrate: basic oil + emulsifier)
  - Coolant solutions (organic or inorganic)

The additives can be classified as:

- Polar additives
- Extreme pressure additives
- Anti-wear additives
- Anti-corrosion additives
- Anti-oxidant additives
- Anti-mist additives, etc.
1.3.1 Oil-based coolants

Creation of separation film (made of base coolant and specific additives) between grinding wheel and workpiece decreases friction, high pressures and temperatures during machining processes.

Oil-based coolants usually consist of 80-95% basic oil and can be divided into four groups [24]:

- Basic oils without additives
- Basic oils with chemically active additives
- Basic oils with surface active additives
- Basic oils with chemically active additives and EP additives (additives that form stable adsorption layers)

The following basic oils are widespread [24]:

- Mineral oils: natural C-H bonds, must be free of harmful aromatic compounds by refining (because of negative health and environmental effects)
- Hydrocrack oils: partly synthetic, low content of aromatic compounds, improved mineral oils
- Polyalphaolefines: fully synthetic oils with branched hydrocarbons, thermally stable
- Synthetic ester: fully synthetic oil of fatty ester acids, thermally stable, biologically decomposable, useable as basic oil and as additive.
In general, and advantage of oil-based coolants over water-based coolants is that they normally provide superior corrosion resistance and lubrication effect. Low viscosity oils have a better crack penetration ability compared to oils with higher viscosity. Increased oil viscosity enables better adhesion and results in producing less oil mist [24].

1.3.2 Water-based coolants

Water-based emulsions or solutions are used if high cooling efficiency and washing away capabilities are needed. The main disadvantage of water-based coolants is susceptibility to leakage oils and microorganisms. Therefore, high maintenance costs cannot be avoided. In addition, the water and oil phases must be separated before disposal. Water-based solutions main ingredients are inorganic and/or organic substances and water. They very seldom contain mineral oils. Further advantages of water-based coolants are high chemical stability and transparency which are important for high cooling efficiency and washing away capability. [24].

Water-based emulsion concentrates are made of 20-70% basic oil (generally mineral oil). For grinding of metals, oil-in-water emulsions are common; the quantity of oil determines the lubrication capability of the emulsion. Usually, oil concentrations in emulsions for grinding operations are between 2% and 15%. Water-based coolants contain up to 20 components. Each of those components can themselves be multicomponent mixtures [24].
1.3.3 Additives

Additives are added to basic fluids to optimize specific types of production process and improve specific coolant properties. Additives can be divided into four groups [24]:

- Enhancers of physical coolant characteristics
- Enhancers of chemical coolant characteristics
- Enhancers of chemical and physical coolant characteristics
- Other additives

In frictional contact with metals, some additives form highly stable compounds either due to their charge polarity or due to chemical reactions at the metal surface. These reactions take place within defined range of temperatures. For that reason, the process temperature is very important influencing factor in the effectiveness of the additive. Polar additive substances (synthetic ester, fatty acids), extreme-pressure (EP) additives (sulfur carrier), anti-wear (AW) additives (phosphorous compounds) and others (anti-corrosion additives, anti-mist additives, antioxidants, emulsifiers, etc.) are all in use as additives [24].

1.4 Fluid delivery problems

One of the most difficult questions to answer in the design of a grinding process is how much grinding fluid flow is required. For cooling, it might be thought that more is better. A large volume of flow helps to keep the bulk temperature of the whole workpiece down and can help to maintain a constant machine temperature. However, pumping large
volumes of fluid at elevated pressures generates heat, wastes power and the fluid itself. Also, too high delivery velocities may lead to the formation of mist, which could become a health hazard. An adequate supply of cooled fluid is ideal.

The models presented in this work have the ability to address fluid delivery problems by including different geometries, grinding parameters, grinding fluid types, etc. into the simulation.

An example where too much flow can be a disadvantage is in internal grinding. The convergent nip and high conformity in internal grinding lead to a hydrodynamic wedge. The fluid pressure builds up as in a hydrodynamic bearing and pushes the grinding wheel away from the workpiece. The long arc of contact in internal grinding means that the grinding fluid is important for lubrication and cooling. A solution is to use a small jet for fluid entering the grinding contact and a higher pressure auxiliary jet for wheel cleaning [1].

For high-removal rates of the chip a large volume of fluid is required. However, for finish grinding to close tolerances, hydrodynamic effects should be minimized. Some users switch the flow rate to a lower setting at the final stage of finishing.

Air entrained around a rotating wheel forms a barrier that impedes fluid delivery. The grinding fluid must first penetrate the air barrier to enter the grinding contact. The air barrier is a low-pressure (sub-ambient) layer of fast-moving air. The entrained velocity at the surface is equal to the wheel velocity. The velocity is smaller farther away from the surface, when the pressure recovers. The fast-moving layer of air surrounding the wheel cannot all pass through the grinding contact and is diverted either to the sides or in the
reverse direction. The same happens with liquid contact. This was shown by Ebbrell et al. [3].

The air barrier is a greater problem with highly porous wheels. A porous wheel pumps air out of the pores. The wheel acts as a pump drawing air in from the sides of the wheels. This is less of a problem with wide non-porous wheels although an air barrier occurs in all grinding wheels. It has been show that using silicone to seal the sides of the wheel reduces the air flow into the air barrier.

Another approach in solving this problem is to physically obstruct the air flow with an air scraper or use the body of the nozzle to obstruct the air flow. It has been shown by several researchers that scraper plates are useful in overcoming the air barrier, particularly at high grinding wheel speeds where the problems become more severe as shown by Trmal and Kaliszer [4]. Positioning the nozzle close to the wheel optimizes fluid delivery and scraper performance.

The usual method advocated for overcoming the problem is to direct the grinding fluid jet at the grinding contact with a velocity approaching or equal to wheel speed (80 % to 100 % of grinding wheel circumferential velocity). The jet should be positioned close to the wheel surface and close to the nip (converging gap at the entry to the grinding contact). It should be directed tangential or almost tangential to the wheel. Too large an angle or distance from the wheel surface causes the fluid to be diverted outwards from the wheel surface or to bounce off it and leads to mist formation [1].

Useful flow rate refers to the fluid that actually enters the grinding contact. It can be measured in an experimental setup by capturing the fluid at the exit from the grinding
contact. Using a conventional flood nozzle, typical useful flow rates were 5-30% of the nozzle flow rate [1,5,6]. With higher jet velocity, higher utilization figures can be obtained. Percentage utilization figures for useful flow rate depend on how well the nozzle is positioned, the jet velocity, the nozzle flow rate and the wheel porosity. The highest percentage utilization figures are obtained when jet velocity is equal to wheel speed [1].

The useful flow rate is greatly different from the nozzle total flow rate as a large proportion of the fluid is dispersed to the sides of the wheel. If the nozzle flow rate is too low, or if the jet is not well positioned, the actual useful flow rate will be substantially lower than the achievable useful flow rate, as shown by Morgan et al. [7]. Increasing the nozzle flow rate excessively is counter-productive as it was found that the inevitable increase in rejected flow interferes with the stream of useful flow.

The surface pores of a grinding wheel act in a similar way to the chambers in a rotary pump. The surface pores at best are only half filled even with a well-directed jet speed equal to wheel speed and adequate nozzle flow. The flow rate required to fill the surface pores depends on the porosity \( \varphi \) of the wheel from manufacturer’s data and the mean depth of the pores, \( h_{pores} \). The depth of the pores can be roughly estimated from the mean grain size or mean grain length for high aspect ratio grains. Allowing for the pores being only half filled, \( Q = 0.5 \cdot \varphi \cdot h_{pores} \cdot b \cdot V_S \), where \( b \) is the width of the grinding contact and \( V_S \) is the wheel speed [1].

The mean depth of the pores is of the same order of magnitude as the abrasive grain size. The porosity of a typical grinding wheel is approximately 30%, where a high
porosity wheel might have 50% porosity or greater. This provides a starting point for estimating the achievable flow rate [1].

1.5 Previous studies of fluid flow in grinding

1.5.1 Analytical & Experimental

Analytical models and experiments regarding the analysis of useful flow rates, fluid flow and heat transfer in the grinding region and its vicinity have been developed.

Gviniaashvili, Woolley and Rowe developed model for flow rate between a rotating grinding wheel and a workpiece [6]. They found that the useful flow that passes through the contact zone is a function of the spindle power for fluid acceleration, wheel speed and delivery-nozzle jet velocity. For the particular grinding wheel and fluid delivery type they introduced two loss coefficients having values less than 1, which must be calibrated. Determination of a suitable value of nozzle outlet gap to achieve a required fluid film thickness in the grinding zone was possible using this model. A guide was given to optimization of the jet velocity in relation to the power required to accelerate the fluid and the particular velocity of the wheel. An example of comparison between experimental data and their results is presented in the Figure 1-1.
Chang Chong-Ching constructed a model based on hydrodynamic pressure and ram pressure effects on flow through grinding [8]. The hydrodynamic pressure was computed using a modified Reynolds equation for porous media with upstream boundary conditions supplied by the ram pressure. His numerical results indicated that for a lower porosity of workpiece the hydrodynamic pressure was higher and the fluid penetrated deeper into the pores of wheel. Also the useful flow rate increased as the porosity of workpiece increased. An example of their results is presented in the figure 1-2.
Figure 1-2 Useful Flowrate vs. Jet Velocity for Various Values of the Porosity of the Workpiece [8].

Ebbrell et al. analyzed the effects of air boundary layer on the grinding process [3]. They showed that the boundary layer reverses direction when approaching the grinding zone, which inhibits the flow of metalworking fluid delivered under flood conditions. CFD was used to model the flow patterns of the boundary layer approaching the minimum gap in order to increase understanding of the flow mechanisms around the grinding zone and improve cutting fluid delivery. The position of fluid delivering nozzle

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was shown to affect the useful flow rate. Results for experimentally measured pressures on the workpiece are shown in the Figure. 1-3

![Experimental Pressure Contours](image)

Figure 1-3 Experimental Pressure Contours [3].

Temperature considerations in grinding were presented in a paper by Liao, Luo and Yang [9]. The researchers have taken into account the thermal effect of the grain-workpiece interface and the shear plane between the workpiece and the chip. It was shown that by taking all of the parameters needed in the model from the experimental results the temperature of the workpiece surface in the grinding zone can be predicted. The conclusion was that the flow rate of the grinding fluid under general grinding conditions was sufficient to cover the thermal boundary layer of the coolant in the grinding zone. By comparison of the predicted workpiece surface temperatures to experimental data for some grinding conditions, good agreement was obtained except for the creep-feed grinding process, when water-based grinding fluid was used. The researchers concluded that the differences between the theoretical values and experimental results are attributed to constant thermal properties and neglect of
transverse conduction in the development of the thermal model. An example of their results is shown in the Figure 1-4.

![Graph showing maximum temperature rise in the fluid](image)

Figure 1-4 Maximum Temperature Rise in the Fluid [9].

Szeri and Chang [24] have developed heat transfer model for thermal analysis of grinding by using volume-averaging techniques to solve heat conduction problem in porous media. They have calculated the maximum temperature in the grinding zone, the workpiece temperature distribution, the fraction of energy going into workpiece, and the grinding energy flux that must be reached to burn. The results were compared to experimental data for two types of coolants, water and oil. Some of the results are presented in the Figure 1-5, showing that maximum grinding zone temperature increases linearly with increasing grinding energy flux,
1.5.2 CFD Studies

Not many CFD investigations of fluid flow and heat transfer in grinding process have been found.
Morgan, Jackson, Wu, Baines-Jones, Batako and Rowe addressed the quantity of fluid required for grinding and the method of application in their paper [7]. Results from their research suggest that supply flow rate needs to be 4 times the achievable useful flow rate. They showed that jet velocity and jet flow rate can be separately specified. Improved system design allows actual useful flow rate to approach achievable useful flow rate. It was also shown that achievable useful flow rate depends on wheel porosity and wheel speed whereas actual useful flow rate depends on nozzle position, design, flow rate and velocity. Experimental methods used in the research were complemented by CFD simulations. They included a 2-D single-phase simulation of air boundary layer forming around the spinning wheel, and a 3-D single-phase simulation of grinding fluid flow inside the delivery nozzle. Simulation results of air pressure distribution around scraper with clockwise wheel rotation are shown in the Fig. 1-6.

Figure 1-6 Simulation Result of Air Pressure Distribution Around Scraper with Clockwise Wheel Rotation [7].
Chapter Two

Analysis and numerical method

Two complex 3-D models were created as a result of this work. No models with the similar level of detail regarding the geometry and physical properties have been found in the literature.

All models were built using a commercial CFD software (ANSYS FLUENT), and correspond to the full grinding geometry (3-D model 1) and respectively to the detailed section of the grinding zone and its immediate vicinity (3-D model 2 and 2-D model).

FLUENT is currently recognized as a mature and dynamic software package, one of the world leaders in CFD platforms. Currently, FLUENT is used as a research tool in a wide variety of domains, such aerodynamics of racing cars, food processing, ship hydrodynamics, heart induced blood flow, or even LASIK surgery. Especially attractive for the problem under study, FLUENT includes a well developed base of models for multiphase flows. However, no publications were found related to the use of FLUENT, or any other commercial CFD package, in the proposed context. By using professionally
tested solvers provided by this platform, this work is able to focus on (i) the components of the physics based model that best represent the complex phenomena under study, and (ii) the analysis, interpretation of the results, and further research using the new model.

2.1 General CFD analysis methodology

CFD is a tool widely used to simulate a wide range of flows in order to aid engineers and scientists in design and analysis. It is attractive for both industry and academia due to the following advantages [41]:

- Less expensive than experiments – ever-decreasing cost of computational power and increasing price of energy and labor goes in favor of CFD
- Faster and less work-intensive than experiments – physical testing usually takes more time and more human physical work
- CFD simulation setup of a range of flows can be closer to real physics and geometry – for example, walls of wind tunnels and holders of wind tunnel models introduce unwanted disturbances to the experimental setup
- Ability to simulate any imaginable type of fluid flow – high hypersonic and high temperature and pressure flows are hard or impossible to study experimentally
- Increasing reliability and accuracy – decades of development of CFD methods and schemes result in better predictions of flows
- Extensive amount of information – contrary to experiments, which extract data from a very limited number of locations in a flow domain, CFD allows
examination of very large number of positions in studied flows; the limit of number of investigated locations is dictated by memory and processing power available.

Along with a large number of advantages, CFD has several disadvantages, such as:

- Some constants and parameters in CFD numerical models cannot be computed, so experiments are needed in order to evaluate their value and then use them in CFD models and schemes
- CFD is still a “black art” – solution accuracy is very dependent on the user’s ability to select and apply appropriate physics and numerics for the model of the flow that is being investigated.

In general, the philosophy of CFD is to replace the continuous physical problem domain with discrete domain using a set of points which is called grid or mesh. In the continuous domain, flow variables are defined at every possible point in the domain. On the other hand, in the discrete domain, flow variables are defined at the grid points, only. The discretized governing equations of the fluid flow and heat transfer are solved at the grid points. For an accurate model, correct geometry, boundary conditions, fluid physical properties, numerical and turbulence parameters have to be identified and applied in precise manner to get meaningful and accurate predictions of flow and heat transfer features.

In all CFD approaches the same following procedure is applied.

1) Preprocessing:
   - Physical bounds of the problem are specified – geometry is defined
• The volume which fluids/solids occupy is divided into a number of discrete cells – mesh is defined
• The physical modeling – the correct physics describing the problem is defined

2) Boundary conditions are defined - this involves specifying the fluid behavior and properties at the boundaries of the problem, and initial conditions if the problem is of transient nature

3) Simulation is run - the simulation is started and the equations are solved iteratively as a steady-state or transient

4) Analysis and visualization of the resulting solution – this step involves usage of a postprocessor.

2.2 Grid generation

Governing equations of fluid flow and heat transfer are nonlinear partial differential equations that have a very limited number of analytical solutions. As a result, in order to analyze fluid flow and heat transfer, flow domains are divided into smaller sub-domains. Sub-domains are made up of geometric primitives like hexahedral and tetrahedral elements in 3D and quadrilateral and triangle elements in 2D. The governing equations are then subjected to a process called discretization, and solved inside each of these sub-domains.

There are several methods to solve the approximate version of the system of equations:

• Finite volume method (used by Ansys FLUENT)
• Finite element method
• Finite difference method
• Boundary element method.

During the analysis a special concern is the proper continuity of solution across the common interfaces between two sub-domains. That is necessary in order to put approximate solutions inside various portions together to give a complete picture of fluid flow and heat transfer in the entire computational domain. The sub-domains are usually called cells or elements. The whole set of cells is called a mesh or grid. Grid generation is a process of generating an appropriate grid. Specialized software exists for the purpose of grid generation. In this work, Ansys Gambit software was used to generate grids for both 2-D and 3-D models.

The most common classification of grids is based upon the connectivity of a grid or on the type of cells the grid is made of.

2.2.1 Structured Grid

“A structured grid is characterized by regular connectivity that can be expressed as a two or three dimensional array” [25]. This puts a limit on the elements that can be used to quadrilaterals in 2D or hexahedra in 3D. The regularity of the connectivity of this type of grid allows conservation of computational memory space since neighborhood relationships are defined by the storage arrangement. Additional classification is made
upon criterion of whether the mesh is conformal or not. For 2-D model presented in this work, structured quadrilateral mesh was used.

2.2.2 Unstructured Grid

“An unstructured grid is characterized by irregular connectivity is not readily expressed as a two or three dimensional array in computer memory” [25]. Therefore, by definition any possible cell type, that a solver is able to use, is allowed. Compared to structured meshes, the memory storage requirements for an unstructured grid can be significantly larger because the neighborhood connectivity must be explicitly stored in computer memory. Due to the complexity of geometry and flow in 3-D part of this work, unstructured tetrahedral meshes were used for 3-D models 1 and 2.

2.2.3 Hybrid Grid

A hybrid grid is a grid composed of both structured and unstructured segments. This type of grid requires data about how the mesh is stored, and used.

There are also grid classifications based on the dimension and type of cells the grid consists of.

According to dimensions of the computational domain, generated grids can be 2-dimensional (2-D) or 3-dimensional (3-D). Usually, cells in 2-D grids are triangles or rectangles, and common in 3-D grids tetrahedral or parallelepiped cells. In 3-D grids, grid nodes are not constrained to lie in a single plane.
The most used 3-D grid cells are:

- Hexahedral
- Tetrahedral
- Pyramidal
- Extruded triangular
- Polyhedral.

All these cells are bounded by faces which correspond to specific 2-D cells.

In CFD simulations, it is often critical that the boundary layer near the wall is resolved in a proper manner. In order to do that, the essential prerequisite is that the grid has to be generated in such a way that it captures boundary layer properly. For flows in which turbulence is present, calculation of the $y^+$ value of the first interior grid point helps in achieving that. This dimensionless distance is defined as

$$y^+ \equiv \frac{u^* \cdot y}{v},$$  \hspace{1cm} (2.1)

where $u^*$ is the so-called “friction velocity” defined as:

$$u^* \equiv \sqrt{\frac{\tau_w}{\rho}}.$$ \hspace{1cm} (2.2)

The wall shear $\tau_w$ usually cannot be calculated until a simulation has been performed. Therefore, it is necessary to estimate a value, and after the simulation is done, check the result.
2.3 Dimensional analysis

In physics, dimensional analysis is a useful tool to determine relations between physical quantities by using their dimensions. The dimension of a physical quantity is the mathematical combination of the elementary physical dimensions which describe it, such as:

- Mass
- Length
- Time
- Electric charge
- Temperature.

Dimensional analysis relies on the fact that a physical law must be independent of the units which are used to measure the physical quantities. So, any meaningful equation must have the same dimensions in the left-hand and right-hand sides. This is called dimensional homogeneity.

Dimensional analysis is regularly used to:

- Check the plausibility of derived equations and computations
- Form reasonable hypotheses about complex physical situations that can be tested by experiment or observations of phenomena
- Categorize types of physical quantities and units based on their relations to or dependence on other units, or their dimensions
Another way of performing dimensional analysis of a flow is to define non-dimensional numbers which represent relations between forces such as:

- Viscous forces
- Gravity
- Inertia
- Buoyancy
- Pressure.

The values of those non-dimensional numbers define type and behavior of a flow. Thus, by analyzing non-dimensional numbers for a particular flow, correct types of solvers and schemes can be used in CFD simulations.

2.3.1 Reynolds number

The Reynolds number, Re, can be defined as the ratio of inertial forces to viscous forces.

For that reason, Re quantifies the relative importance of these two types of forces for given flow conditions. The mathematical expression for Reynolds number is [26]:

\[
\text{Re} = \frac{\rho U L}{\mu} = \frac{U L}{\nu},
\]

(2.3)

where:
- U is the characteristic velocity of the flow
- L is a characteristic linear dimension
- \( \mu \) is the dynamic viscosity of the fluid
- \( \nu \) is the kinematic viscosity of the fluid
- \( \rho \) is the density of the fluid.

The point of using Reynolds number is when performing dimensional analysis of fluid dynamics problems. It can be used to determine dynamic similitude between different experimental cases performed. \( Re \) is also used to characterize different flow regimes, for example laminar or turbulent flow. Laminar flow occurs at low Reynolds numbers, because of the dominance of viscous forces. It is characterized by smooth, constant fluid motion. Inertia tends to produce flow instabilities and chaotic vortical motion of different length and time scales. If instabilities are present, and the Reynolds number is high enough, a transition between laminar and turbulent flow occurs. Turbulent flow is dominated by inertial forces, so it’s important to state that turbulence is an inviscid phenomenon which occurs in viscous flows.

Reynolds number can be defined for a number of different flows and geometries. Dimensions and velocities used to define Reynolds number depend on convention. For an example, a radius or diameter are equally valid for spheres or circles, but one of them is chosen by convention. For aircraft or ships, the length or width can be used. For flow in a pipe the internal diameter is usually used. Other shapes, such as rectangular pipes or non-spherical objects, have an equivalent diameter or radius defined. The velocity is also a matter of convention in some situations.
In a turbulent flow, there is a range of length and time scales of the unsteady fluid motion. The size of the largest eddies present in the flow field is determined by the overall geometry and size of the flow domain. For instance, in turbulent boundary layer, the largest scales of fluid motion are as big as the thickness of the boundary layer itself. The size of the smallest eddies is determined by the Reynolds number. As the Reynolds number increases, smaller and smaller eddy sizes are present in the flow. Therefore, the Reynolds number is an indicator of the range of scales in the flow - higher Reynolds numbers result in greater the range of scales. Why is this so? A large Reynolds number indicates that viscous forces have negligible importance at large scales of the flow. In that case, inertial forces dominate significantly over viscous forces, so the largest eddies of fluid flow are not damped, because the viscosity is not high enough to dissipate their motion. The kinetic energy of the flow cascades from the large eddies to progressively smaller eddies until a length scale is reached for which the viscosity becomes important – orders of magnitude of inertia and viscosity become comparable. At these small length scales, called Kolmogorov scales, the dissipation of energy by viscous forces takes place. Therefore, the Reynolds number shows the ratio of the largest eddies of the turbulent flow to the smallest eddies.

To summarize properties of turbulent flow, several characteristics of that type of fluid flow can be listed. Turbulence is:

- Unsteady
- Vortical, comprised of eddies with a range of sizes
- 3-D only, unsteady velocities in all three dimensions, all three components of vorticity
- Chaotic (not random!) – highly sensitive to initial conditions, but it does have a structure
- An inviscid phenomenon occurring in viscous flows
- Diffusive - it increases mixing rates of momentum, heat and mass transfer compared to molecular viscous terms (molecular laminar processes)
- Dissipative: the turbulent eddies take kinetic energy out of the flow and, in the end, convert it into heat when the eddies dissipate at smallest length scales
- A continuum phenomenon
- A feature of the flow, not of the fluid itself.

The Reynolds number regime for which turbulence occurs is:

- For internal flows: above Reynolds number of about 2300
- For external flows, such as flow over a plate or circular cylinder: above Reynolds numbers of about $5 \cdot 10^5$.

In 2-D and 3-D models used in this work, type and characteristics of the flow at the liquid inlet which brings the metalworking fluid to the computational domain, and of the flow in the domain itself have to be determined. The flows depend on the Reynolds number, and it has to be checked if the Reynolds number is high enough for turbulent flow. For the simulations presented in this work Reynolds number at the inlet (internal flow) goes up to 30 000, which is well inside the turbulent region. The Reynolds numbers in the domain itself (external flow) goes up to 1.3 million which also indicates presence of the turbulence and implies a must of use of a turbulence model in simulations.
The liquid inlet boundary conditions require turbulence intensity and length scale specification.

The turbulence intensity at the core of a fully-developed duct flow can be estimated from the following formula derived from an empirical correlation for pipe flows [10]:

\[ I \equiv \frac{u'}{u_{avg}} = 0.16 \cdot \frac{1}{\text{Re}_{D_h}^{0.16}}, \quad (2.4) \]

where:
- \( u_{avg} \) is average velocity inside the nozzle
- \( u' \) is the unsteady component of the velocity
- \( \text{Re}_{D_h} \) is Reynolds number determined by the hydraulic diameter of the pipe.

The turbulence length scale used in the Eq. (2.4), \( l \), is defined as a physical quantity related to the size of the large eddies that contain most of the energy in turbulent flows. An approximate relationship between \( l \) and the physical size of the pipe is [10]:

\[ l = 0.07 \cdot D, \quad (2.5) \]

where \( D \) the diameter of the pipe. The factor of 0.07 is based on the maximum value of the mixing length in fully-developed turbulent pipe flow, where \( D \) is the diameter of the pipe [10].
2.3.2 Mach Number

Mach number is defined as the ratio between the speed of an object moving through a fluid and the speed of sound in that fluid for its particular physical conditions, such as temperature and pressure. It delineates different fluid flow regimes related to the compressibility effect. The mathematical definition of Mach number is [26]:

\[ M \equiv \frac{U}{a}, \quad (2.6) \]

where:

- \( M \) is the Mach number
- \( U \) is the relative velocity of the source to the fluid medium
- \( a \) is the speed of sound in the medium - the rate of propagation of small disturbance pressure pulses through the fluid.

The speed of sound is calculated as [26]:

\[ a = \sqrt{\gamma \cdot R \cdot T}, \quad (2.7) \]

where:

- \( \gamma \) is specific heat ratio
- \( R \) is the molar gas constant (equal to 8.3145 \( \frac{J}{mol \cdot K} \))
- \( T \) is the absolute temperature [K]
When performing a CFD analysis with gas flow, compressibility effects must be considered. Those effects represent significant density changes caused by the flow. Compressibility starts to become significant when the flow velocity is a significant fraction of the speed of sound of the fluid, i.e. when the Mach number of the flow exceeds 0.3 [26].

In the fluid flow problem presented in this work, maximum velocities were up to Mach 0.35, present in a very small region only, but in the majority of cases, velocities were about an order of magnitude lower. Therefore, it was decided to use incompressible pressure based solver.

2.3.3 Weber number

The Weber number is a dimensionless number in that is used in analysis of fluid flows where there is an interface between two different fluids, particularly for multiphase flows with highly curved surfaces. It defines the relative importance of the fluid's inertia compared to the fluid's surface tension.

\[
We = \frac{\rho \cdot U^2 \cdot L}{\sigma},
\]

(2.8)

where:

- \( \rho \) is the density of the fluid
- \( U \) is the velocity of the fluid
- \( L \) is the characteristic length
• \( \sigma \) is the surface tension.

The influence of Weber number is large only if it is of order of one or less. That usually occurs when the surface curvature is comparable in size to the liquid depth. On the other hand, if Weber number is large, surface tension effects may be ignored.

The fluid flow in grinding involves multiphase interaction between metalworking fluid and surrounding air. Therefore it is necessary to calculate representative Weber numbers in order to determine importance of surface tension effects.

In the simulations performed in this work local Weber number, calculated based on the thickness of the grinding region, ranges from 20 to 800. Global Weber number, calculated based on the size of the domain, was up to 32000000. Therefore, calculations indicate that surface tension effects should not be influential. That is proved by parametric study of surface tension influence on flow and heat transfer parameters in this work (Chapter 3.2.6.6).

2.4 Multiphase models

There are many flows encountered in nature and technology which have a mixture of different fluid phases. In physics, phases of matter are: gas, liquid, and solid. But, in fluid mechanics, the concept of phase in a multiphase flow is used in a somewhat broader sense. A phase can be defined as: “an identifiable class of material that has a particular inertial response to and interaction with the flow and the potential field in which it is immersed” [10]. Therefore, solid particles of different size, which are made of the same
material, can be treated as distinct phases because each set of particles of the same size has a similar dynamical reaction to the flow field.

2.4.1 Multiphase Flow Regimes

Regimes of multiphase flow can be grouped into four types [10]:

- Gas-liquid or liquid-liquid flows
- Gas-solid flows;
- Liquid-solid flows
- Three-phase flows.

2.4.1.1 Gas-Liquid or Liquid-Liquid Flows

The following regimes are gas-liquid or liquid-liquid flows [10]:

- Bubbly flow - the flow of discrete gaseous or fluid bubbles in a continuous fluid
- Droplet flow - the flow of discrete fluid droplets in a continuous gas
- Slug flow - the flow of large bubbles in a continuous fluid
- Stratified/free-surface flow - the flow of immiscible fluids separated by a clearly-defined interface.
2.4.1.2 Gas-Solid Flows

The following regimes are gas-solid flows [10]:

- **Particle-laden flow** - the flow of discrete particles in a continuous gas
- **Pneumatic transport** - a flow pattern that depends on factors such as solid loading, Reynolds numbers, and particle properties; typical patterns are dune flow, slug flow, packed beds, and homogeneous flow
- **Fluidized bed** - consists of a vertical cylinder containing particles, into which a gas is introduced through a distributor. The gas rising through the bed suspends the particles. Depending on the gas flow rate, bubbles appear and rise through the bed, intensifying the mixing within the bed.

2.4.1.3 Liquid-Solid Flows

The following regimes are liquid-solid flows [10]:

- **Slurry flow** - the transport of particles in liquids. The fundamental behavior of liquid-solid flows varies with the properties of the solid particles relative to those of the liquid. In slurry flows, the Stokes number is normally less than 1. When the Stokes number is larger than 1, the characteristic of the flow is liquid-solid fluidization
- **Hydrotransport** - describes densely-distributed solid particles in a continuous liquid
• Sedimentation - describes a tall column initially containing a uniform dispersed mixture of particles.

2.4.2 Examples of Multiphase Systems

Some examples of each multiphase flow regime are [10]:

• Bubbly flow examples include absorbers, aeration, air lift pumps, cavitation, evaporators, flotation, and scrubbers
• Droplet flow examples include absorbers, atomizers, combustors, cryogenic pumping, dryers, evaporation, gas cooling, and scrubbers
• Slug flow examples include large bubble motion in pipes or tanks
• Stratified/free-surface flow examples include sloshing in offshore separator devices and boiling and condensation in nuclear reactors
• Particle-laden flow examples include cyclone separators, air classifiers, dust collectors, and dust-laden environmental flows
• Pneumatic transport examples include transport of cement, grains, and metal powders
• Fluidized bed examples include fluidized bed reactors and circulating fluidized beds
• Slurry flow examples include slurry transport and mineral processing
• Hydrotransport examples include mineral processing and biomedical and physiochemical fluid systems
• Sedimentation examples include mineral processing.
2.4.3 Method of Choosing Appropriate Multiphase Model

Initial step in solving a multiphase fluid flow problem is to find out which of the flow regimes provides adequate guidelines to determine appropriate models for each flow regime, and how to resolve the degree of interphase coupling for multiphase flows involving bubbles, droplets, or particles, and the adequate model for different amounts of coupling [10].

2.4.4 Approaches to Multiphase Modeling

New methods in CFD have made further insight into the dynamics of multiphase fluid flows possible. At present, there are two different approaches for the numerical calculation of multiphase fluid flows:

- Euler-Lagrange approach
- Euler-Euler approach.

In the Euler-Euler approach, the different fluid phases have mathematical treatment as interpenetrating continua. Because the volume of a single phase cannot be occupied by any other phase, the concept of “phasic” volume fraction is used. Therefore, it is assumed that volume fractions are continuous functions of both space and time and the total sum is equal to one. Equations of conservation for every phase are derived in order to obtain a set of equations that have similar structure for all phases. The equations are closed by method of providing specific constitutive relations which are obtained from experiments, or by application of kinetic theory [10].
In common use there are three different Euler-Euler multiphase models [10]:

- The volume of fluid (VOF) model
- The mixture model
- The Eulerian model.

2.4.4.1 The VOF Model

The VOF model is a type of a surface-tracking technique which is applied to a fixed Eulerian grid. It was made for simulations of two or more immiscible fluids when the position of the fluid interface is of interest. In this model, there is a single set of momentum equations which is shared by all fluids. The volume fraction of every fluid in each computational cell is tracked all over the domain. Most common applications of the VOF model are in [10]:

- Stratified flows
- Free-surface flows
- Filling, sloshing
- The motion of large bubbles in a liquid
- The motion of liquid after a dam break
- The prediction of jet breakup (surface tension)
- The steady or transient tracking of any liquid-gas interface.
2.4.4.2 The Mixture Model

The mixture model was made for flows of two or more fluid or particulate phases. This model shares a characteristic with the Eulerian model - the phases are treated as interpenetrating continua. The mixture model solves the mixture momentum equation and specifies relative velocities in order to describe the dispersed phases. It can be used without relative velocities approach for the dispersed phases in order to model homogeneous multiphase flow.

Most common applications of the mixture model are in [10]:

- Particle-laden flows with low loading
- Bubbly flows
- Sedimentation
- Cyclone separators.

2.4.4.3 The Eulerian Model

The Eulerian model is the most complex of the Euler-Euler multiphase models. This model solves a set of momentum and continuity equations for every phase. Coupling is achieved by use of the pressure and interphase exchange coefficients. The way of handling the coupling depends on the type of phases involved. Exchange of momentum between different phases is dependent on the type of mixture being modeled. Common applications of the Eulerian multiphase model are in [10]:

- Bubble columns
• Risers
• Particle suspension
• Fluidized beds.

2.4.4.4 Comparison of Different Multiphase Models

When the flow regime that is the best representation of investigated multiphase flow is determined, the appropriate multiphase model has to be selected. The following guidelines are usually used [10]:

• For bubbly, droplet, and particle-laden flows in which the phases mix and/or dispersed-phase volume fractions exceed 10%, it is recommended to use the mixture model or the Eulerian model.
• For slug flows, use of the VOF model is recommended.
• For stratified/free-surface flows it is recommended to use the VOF model.
• For pneumatic transport it is recommended to use the mixture model for homogeneous flow or the Eulerian model for granular flow.
• For fluidized beds, the Eulerian model for granular flow is recommended.
• For slurry flows and hydrotransport, the mixture or Eulerian model is recommended.
• For sedimentation recommendation is to use the Eulerian model.
• For general, complex multiphase flows which include multiple flow regimes the multiphase model that is most appropriate for the most important aspect of the
flow should be applied; the downside of this approach is that accuracy might be impaired since the used model is valid for only part of the flow.

In order to choose between the mixture model and the Eulerian model, there are some guidelines [10]:

- If there is a broad distribution of the dispersed phases, it is recommended that the mixture model is better because it is less computationally expensive; if there is high concentration of dispersed phases just in some parts of the domain the Eulerian model should be used instead.
- If laws that describe drag between the phases, the Eulerian model is usually more accurate compared to the mixture model; on the other hand, if there is no knowledge of the interphase drag laws the mixture model should be used; for majority of cases that include spherical particles Schiller-Naumann or Morsi-Alexander laws are quite adequate.
- In order to solve a simpler problem, that requires less computational power, the better option is to use mixture model, because it solves a smaller number of equations compared to the Eulerian model; on the other hand, if accuracy is preferable over low computational effort, the Eulerian model should be applied.

2.4.5 Stability and Convergence

There are a lot of difficulties in related to the process of solving a multiphase system. Because of that, some stability or convergence problems can be encountered. In the case
of time-dependent problems, recommendation is that a few iterations with a small time step are performed first. The time step size should be at least an order of magnitude smaller than the characteristic time of the flow in question. The time step size can be increased after performing a few time steps. If steady calculations are being performed, recommendations are that simulation should start with a small under-relaxation factor for the volume fraction. Another recommendation is to start the simulation with non-zero volume fraction. To start with a mixture multiphase calculation first, and then change the model to the Eulerian can increase stability of calculations.

2.4.6 Volume of Fluid Model Theory

2.4.6.1 Overview of the VOF Model

This model can include simulations with two or more immiscible fluids. VOF multiphase model solves a single set of momentum equations, and tracks the volume fraction of each fluid phase throughout the domain.

Common applications of VOF multiphase model are:

- The prediction of jet breakup
- The motion of large bubbles in a liquid
- The motion of liquid after a dam break
- The steady or transient tracking of any liquid-gas interface.
2.4.6.2 Steady-State and Transient VOF Calculations

The VOF can be used to compute both time-dependent and steady-state solutions. Performing steady-state VOF calculations is adequate only when the solution of the problem is independent of the initial conditions and distinct inflow boundaries exist for the individual phases. A common example of steady-state calculation is the flow of water in a channel with air on the top and a separate air inlet. The VOF model relies on the detail that two or more fluids are not interpenetrating. For every distinct phase that is added to the model, a variable is introduced. That variable is the volume fraction of the phase in the computational cell. The rule is that in every control volume the volume fractions of all phases have to sum to unity. The fields of different variables and properties are shared by all phases and represent volume-averaged values. Therefore, the variables and properties in any computational cell are purely representative of only one of the phases, or representative of a mixture of the phases. That depends on the volume fraction values. So, if the $q^{th}$ fluid's volume fraction in a computational cell is denoted as $\alpha_q$, there are three possible conditions [10]:

- $\alpha_q = 0$: The cell is empty (of the $q^{th}$ fluid).
- $\alpha_q = 1$: The cell is full (of the $q^{th}$ fluid).
- $0 < \alpha_q < 1$: The cell contains the interface between the $q^{th}$ fluid and one or more other fluids.

Based on the local value of $\alpha_q$, the adequate properties and variables are assigned to every control volume inside the domain.
2.4.6.3 Volume Fraction Equation

By solving the continuity equation for the volume fraction of one or more phases the tracking of the phase interfaces is accomplished. For the $q^{th}$ phase, continuity equation has the following form [10]:

$$
\frac{1}{\rho_q} \left[ \frac{\partial}{\partial t} (\alpha_q \cdot \rho_q) + \nabla \cdot (\alpha_q \cdot \rho_q \cdot \vec{v}_q) \right] = S_{\alpha_q} + \sum_{p=1}^{n} \left( \dot{m}_{pq} - \dot{m}_{qp} \right),
$$

where:

- $\dot{m}_{qp}$ is the mass transfer from phase $q$ to phase $p$
- $\dot{m}_{pq}$ is the mass transfer from phase $p$ to phase $q$.

By default, the source term on the right-hand side of Eq. (2.9), $S_{\alpha_q}$, is zero. But constant or user-defined mass source can be specified for each phase. The volume fraction equation is not solved for the primary phase, but the primary-phase volume fraction is computed according to the following constraint [10]:

$$
\sum_{q=1}^{n} \alpha_q = 1.
$$

Implicit or explicit time discretizations can be utilized to solve the volume fraction equation.
2.4.6.4 The Implicit Scheme

If the implicit scheme is used as time discretization, following finite-difference interpolation schemes can be used in order to obtain the face fluxes for all cells, including those near the interface:

- QUICK
- First Order Upwind
- Second Order Upwind
- The Modified HRIC.

The discretized equation is [10]:

\[
\frac{\alpha_q^{n+1} \cdot \rho_q^{n+1} - \alpha_q^n \cdot \rho_q^n}{\Delta t} \cdot V + \sum_f \left( \rho_f^{n+1} \cdot U_f^{n+1} \cdot \alpha_{q,f}^{n+1} \right) = \left[ S_{\alpha_q} + \sum_{p=1}^n \left( \dot{m}_{pq} - \dot{m}_{qp} \right) \right] \cdot V
\] (2.11)

Because Eq. (2.11) requires values of volume fraction at the current time step (instead at the previous step, as for the explicit scheme), the procedure is to solve a standard scalar transport equation iteratively for every secondary-phase volume fraction at every time step. This scheme can be used for both time-dependent and steady-state calculations [10].
2.4.6.5 The Explicit Scheme

The explicit scheme uses finite-difference interpolation schemes are applied to the volume fraction values that were calculated at the previous time step. The discretized equation is [10]:

$$\frac{\alpha_{q}^{n+1} \cdot \rho_{q}^{n+1} - \alpha_{q}^{n} \cdot \rho_{q}^{n}}{\Delta t} \cdot V + \sum_{f} \left( \rho_{q}^{n} \cdot U_{f}^{n} \cdot \alpha_{q,f}^{n} \right) = \left[ S_{\alpha_{q}} + \sum_{p=1}^{n} (\dot{m}_{pq} - \dot{m}_{qp}) \right] \cdot V,$$

where:

- \( n+1 \) is the index for the current time step
- \( n \) is the index for previous time step
- \( \alpha_{q,f} \) is the face value of the q\(^{th}\) volume fraction, that is calculated from the first or second-order upwind, QUICK, modified HRIC, or CICSAM scheme
- \( V \) is the volume of cell
- \( U_{f} \) is the volume flux through the face, based on normal velocity.

This kind of formulation does not need that the transport equation is iteratively solved during each time step. If the explicit scheme is used for time discretization, interpolation of the face fluxes can be done using interface reconstruction or using a finite volume discretization scheme. Common reconstruction based schemes are:

- Geo-Reconstruct
- Donor-Acceptor.

The discretization schemes usually used with explicit scheme for VOF multiphase model are:
• First Order Upwind
• Second Order Upwind
• CICSAM
• Modified HRIC
• QUICK.

2.4.6.6 The Geometric Reconstruction Scheme

In this scheme, interpolation schemes are used to find the face fluxes every time a cell is completely filled with one phase only. The geometric reconstruction scheme is used if a computational cell is close to the interface between two phases.

The interface between fluids is represented using a piecewise-linear approach. For general unstructured meshes this scheme is usually the most accurate. In the work of Youngs generalization of this scheme for unstructured meshes can be found [27]. The generalization assumes that the interface between two fluids has a linear slope within every cell. Then, it uses the linear shape for computing the advection of fluid through the computational cell faces.

In the first step, this reconstruction scheme calculates the relative position of the linear interface compared to the position of the center of every partially-filled cell. That calculation is done based on information regarding the volume fraction and its derivatives in the cell. The next step is to calculate the advecting quantity of fluid through each face. That is done by using the calculated linear interface representation and data about the normal and tangential velocity distribution on the cell face. The final step is to compute
the volume fraction in every cell. It is achieved by using the flux balance calculated during the second step.

2.4.6.7 The Donor-Acceptor Scheme

In this scheme, the interpolation schemes are used to compute the face fluxes every time a computational cell is completely filled with one phase only. When the computational cell is close to the interface between two phases, a "donor-acceptor" numerical scheme is applied in order to find the amount of fluid that advects through the cell face [28]. The donor-acceptor scheme identifies one cell as a donor of an amount of one fluid phase and another, neighboring cell is identified as the acceptor of that same amount of fluid phase. It is also used to prevent numerical diffusion at the phase interface. The minimum of two specific properties limits the amount of fluid from one phase that can be convected across a cell boundary. Those properties are:

- The filled volume in the donor cell
- The free volume in the acceptor cell.

To determine the face fluxes the orientation of the interface is also used. The interface orientation can be horizontal or vertical. That depends on the direction of gradient of the volume fraction of the q\textsuperscript{th} phase inside the cell, and that of the neighbor cell that shares the face. The flux values are obtained according to the orientation of the interface and the motion of the interface by pure upwinding, pure downwinding, or some combination of those methods [10].
2.4.6.8 The CICSAM Scheme

The Compressive Interface Capturing Scheme for Arbitrary Meshes (CICSAM) scheme is a type of high resolution differencing schemes. It is based on the work of Ubbink [29]. The CICSAM scheme is especially fitting for multiphase flows with high viscosity ratio between the phases, and offers the advantage that reflects in producing an interface which is almost as sharp as the geometric reconstruction scheme [10].

2.4.6.9 Material Properties

The presence of the phases in every control volume determines the properties that appear in the transport equation. For example, in a two-phase flow, the phases are denoted by the subscripts 1 and 2, and the volume fraction of the second of these is being tracked, therefore the density in every cell is given by [10]:

$$\rho = \alpha_2 \cdot \rho_2 + (1 - \alpha_2) \cdot \rho_1. \quad (2.13)$$

General form, for an n-phase system, of the volume-fraction-averaged density is [10]:

$$\rho = \sum \alpha_q \rho_q. \quad (2.14)$$

All other fluid properties can be calculated in this way.
2.4.6.10 Momentum Equation

Only one momentum equation is solved throughout the computational domain, and the phases share the resulting velocity field. The momentum equation depends on the volume fractions of all phases with respect to the properties $\rho$ and $\mu$ [10]:

$$\frac{\partial}{\partial t}(\rho \cdot \ddot{v}) + \nabla \cdot (\rho \cdot \ddot{v} \cdot \ddot{v}) = -\nabla p + \nabla \cdot \left[ \mu \cdot (\nabla \ddot{v} + \nabla \ddot{v}^T) \right] + \rho \cdot \ddot{g} + \ddot{F}.$$  \hspace{1cm} (2.15)

In cases where there are large velocity differences between the phases, the accuracy of the velocities computed close to the interface can be negatively affected. That limitation is the result of shared-fields approximation [10].

Another problem is that if the viscosity ratio of fluids present in the simulation is more than 1000, convergence difficulties may happen. CICSAM scheme is particularly effective in simulating multiphase flows with high ratios of viscosities between the phases and solves the problem of poor convergence [10].

2.4.6.11 Energy Equation

The energy equation is shared among the phases, too [10]:

$$\frac{\partial}{\partial t}(\rho \cdot E) + \nabla \cdot (\ddot{v} \cdot (\rho \cdot E + p)) = \nabla \cdot (k_{\text{eff}} \cdot \nabla T) + S_h.$$  \hspace{1cm} (2.16)
The VOF model considers that energy, $E$, and temperature, $T$, are mass-averaged variables [10]:

$$E = \frac{\sum_{q=1}^{n} \alpha_q \cdot \rho_q \cdot E_q}{\sum_{q=1}^{n} \alpha_q \cdot \rho_q},$$  

(2.17)

where $E_q$ for every phase is based on the specific heat of that particular phase and the temperature that is shared.

Phases share the properties $\rho$ and $k_{\text{eff}}$ (effective thermal conductivity). The source term, $S_h$, includes contributions from radiation, and any other present volumetric heat source.

The accuracy of the temperature close to the interface is can be poor in cases where there is a large temperature difference between the fluid phases. Accuracy and convergence problems can also happen when the fluid properties vary by several orders of magnitude. Such large discrepancies in properties lead to sets of equations that contain anisotropic coefficients. That can lead to convergence and accuracy limitations.

2.4.6.12 Surface Tension and Wall Adhesion

The effects of surface tension along the interface between each pair of phases can be included in VOF multiphase model. Additional specification of the contact angles between the phases and the walls can augment the model. The FLUENT solver also includes the additional tangential stress terms that arise due to the variation in surface
tension coefficient. That results in so-called Marangoni convection. Conditions in which variable surface tension coefficient effects can be important are when gravity is low or absent [10].

Surface tension is a physical phenomenon that is a result of attractive forces between molecules in a fluid. A good example is an air bubble in water. Inside the bubble, the sum of forces that act on a molecule due to the neighboring molecules is zero. At the surface, there is different situation - the net force is directed radially inward, so the combined effect of the radial components of force across the whole spherical surface is that the surface contracts. That increases the pressure on the concave side of the surface. The result is that surface tension force acts only at the surface and is required to maintain equilibrium in such cases. Surface tension balances the radial inward inter-molecular attractive force with the radial outward pressure gradient force across the surface. If two fluids are separated in a region, but one of the fluids is not in the form of bubbles of spherical shape, the surface tension force minimizes free energy by mechanism of decreasing the area of the interface.

One of the most used surface tension models is the continuum surface force (CSF) model of Brackbill et al. [30]. By applying this model, surface tension is added to the VOF computation. That results in an additional source term in the momentum equation. The basis of the source term can be explained by considering a special case. In that case, there is constant surface tension coefficient along the surface; only the forces which are normal to the fluid interface are considered. The pressure drop across the surface is dependent on two factors: the surface tension coefficient, σ, and the curvature of the surface (measured defined by two radii in orthogonal directions, R$_1$ and R$_2$).
The pressure drop is [10]:

\[ p_2 - p_1 = \sigma \cdot \left( \frac{1}{R_1} + \frac{1}{R_2} \right), \]  

(2.18)

where \( p_1 \) and \( p_2 \) are the pressures in the two fluids on both sides of the interface.

It is usual that the CSF model the surface curvature is calculated from local gradients in the surface normal at the interface. The surface normal, \( n \), that is defined as the gradient of quantity \( \alpha_q \), which is the volume fraction of the \( q^{th} \) phase [10]:

\[ n = \nabla \alpha_q. \]  

(2.19)

Parameter \( \kappa \) is curvature. I can be defined as the divergence of the unit normal, \( \hat{n} \) [30]:

\[ \kappa = \nabla \cdot \hat{n}, \]  

(2.20)

where \( \hat{n} \equiv \frac{n}{|n|} \).

The surface tension effect can be described including the pressure jump across the surface. Force that acts on the surface can be transformed to a volume force by using the divergence theorem. So, this volume force is the source term that is added to the momentum equation. The force has the following form [10]:

\[ F_{vis} = \sum_{pairs \atop \bar{i}, \bar{j} < \bar{j}} \sigma_{\bar{i}\bar{j}} \cdot \frac{\alpha_i \cdot \rho_i \cdot \kappa_j \cdot \nabla \alpha_j + \alpha_j \cdot \rho_j \cdot \kappa_i \cdot \nabla \alpha_i}{\frac{1}{2} \left( \rho_i + \rho_j \right)} \].  

(2.21)
A smooth superposition of forces close to computational cells in which more than two phases are present is possible with this expression. In the case when just two phases are present in a computational cell, then $\kappa_i = -\kappa_j$ and $\nabla \alpha_i = -\nabla \alpha_j$. Therefore, Eq. (2.21) simplifies to [10]:

$$F_{vol} = \sigma_{ij} \cdot \rho \cdot \kappa_i \cdot \nabla \alpha_i \cdot \frac{1}{2} \left( \rho_i + \rho_j \right),$$

(2.22)

where $\rho$ is the volume-averaged density computed using Eq (2.13). Equation (2.22) shows proportionality if surface tension source term to the average density in the cell.

It should be mentioned that computations of surface tension effects on grids composed of triangular or tetrahedral cells is less accurate compared to grids made of quadrilateral or hexahedral cells. Therefore, regions of the flow where surface tension effects have high importance should be meshed using quadrilateral or hexahedral cells.

The weight of effects of surface tension can be determined according to the value of two dimensionless numbers: the Reynolds number, Re, and the capillary number, Ca; or the Reynolds number, Re, and the Weber number, We [10]. If $Re \ll 1$, the quantity of interest is the capillary number:

$$Ca = \frac{\mu \cdot U}{\sigma},$$

(2.23)

and if $Re \gg 1$, the quantity of interest is the Weber number. Surface tension effects can be neglected if $Ca \gg 1$ or $We \gg 1$. In this work, Reynolds number is much larger that 1
for every simulation case, so Weber number was considered as the important dimensionless number in order to study importance of surface tension effects.

In FLUENT simulations performed in this work, a wall adhesion angle in conjunction with the surface tension model was specified. That numerical model is based on the work done by Brackbill et al. [30]. Instead of imposing this boundary condition at the wall itself, the use of the contact angle that the fluid is assumed to make with the wall is to adjust the surface normal in computational cells close to the wall. That boundary condition is called dynamic boundary condition. It results in the fine-tuning of the curvature of the surface close to the wall.

If the contact angle at the wall is denoted as $\theta_w$, then the surface normal at the live cell right next to the wall is [10]:

$$\hat{n} = \hat{n}_w \cdot \cos \theta_w + \hat{i}_w \cdot \sin \theta_w,$$

(2.24)

where $\hat{i}_w$ and $\hat{n}_w$ are the unit vectors tangential and normal to the wall, respectively. From the combination of the contact angle with the normally calculated surface normal one cell away from the wall the local curvature of the surface is determined. This curvature is then used in order to adjust the body force term in the surface tension computation.
2.4.6.13 Open Channel Flow

The FLUENT software is able to model the effects of open channel flow by using the open channel boundary condition and the VOF model. In open channel flows there is a free surface between the flowing fluid (usually liquid) and the fluid which is above it (usually the atmosphere). In cases like that, the propagation of waves and free surface behavior can be important. Therefore, fluid flow in open channels is governed by the forces of gravity and inertia, generally.

Dimensionless number that characterizes open channel flows is Froude Number. It is defined as the ratio of forces of inertia and hydrostatic force [10]:

$$Fr = \frac{V}{\sqrt{g \cdot y}},$$

(2.25)

where:

- $V$ is the characteristic velocity magnitude
- $g$ is gravity
- $y$ is a length scale - the distance from the bottom of the channel to the free surface.

The denominator in Eq. (2.25) is the speed of propagation of the wave. The fixed observer sees the wave speed of [10]:

$$V_w = V \pm \sqrt{g \cdot y}.$$  

(2.26)
Ranges of the Froude number delineate different open channel flows into the following three types [10]:

- If \( Fr < 1 \), i.e. \( V < \sqrt{g \cdot y} \), (therefore \( V_w < 0 \) or \( V_w > 0 \)), the flow is called subcritical - disturbances can travel upstream as well as downstream. In such case, downstream conditions are able to affect the flow upstream.

- If \( Fr = 1 \) (therefore \( V_w = 0 \)), the flow is called critical - upstream propagating waves remain stationary. In such case, the character of the flow changes.

- If \( Fr > 1 \), i.e. \( V > \sqrt{g \cdot y} \), (thus \( V_w > 0 \)), the flow is known to be supercritical where disturbances cannot travel upstream - downstream conditions do not affect the flow upstream. In this work, the characteristic velocity, based on the metalworking inlet velocity, is usually about two orders of magnitude larger than the term \( \sqrt{g \cdot y} \), and therefore is supercritical.

2.4.6.14 Upstream Boundary Conditions

There exist two options that are available in FLUENT software for the upstream boundary condition for open channel flows [10]:

- pressure inlet
- mass flow rate
2.4.6.14.1 Pressure Inlet

The total pressure $p_0$ at the inlet is given as [10]:

$$p_0 = \frac{1}{2} \cdot (\rho - \rho_0) \cdot V^2 + (\rho - \rho_0) \cdot |\mathbf{g}| \cdot (\hat{\mathbf{g}} \cdot (\mathbf{b} - \mathbf{a})),$$

(2.27)

where:

- $\mathbf{a}$ and $\mathbf{b}$ are the position vectors of any point on the free surface and the face centroid, respectively; it is assumed that the free surface is horizontal and normal to the direction of gravity
- $\mathbf{g}$ is the gravity vector,
- $|\mathbf{g}|$ is the gravity magnitude
- $\hat{\mathbf{g}}$ is the unit vector of gravity
- $V$ is the velocity magnitude
- $\rho$ is the density of the mixture in the cell
- $\rho_0$ is the reference density.

According to this, the dynamic pressure $q$ is calculated as [10]:

$$q = \frac{\rho - \rho_0}{2} \cdot V^2,$$

(2.28)

and the static pressure $p_s$ is calculated as [10]:

$$p_s = (\rho - \rho_0) \cdot |\mathbf{g}| \cdot (\hat{\mathbf{g}} \cdot (\mathbf{b} - \mathbf{a})).$$

(2.29)
The Eq. (2.29) can be further expanded to [10]:

\[ p_s = (\rho - \rho_0) \cdot |\vec{g}| \cdot \left( (\hat{\vec{g}} \cdot \hat{\vec{b}}) + y_{local} \right), \tag{2.30} \]

where the distance from the free surface to the reference position, \( y_{local} \), is defined as [10]

\[ y_{local} = - (\vec{a} \cdot \hat{\vec{g}}). \]

### 2.4.6.14.2 Mass Flowrate

In the open channel flow, the mass flow rate for each phase is defined as [10]:

\[ \dot{m}_{phase} = \rho_{phase} \cdot (Area_{phase}) \cdot (Velocity). \tag{2.31} \]

According to FLUENT recommendations [10], in cases when mass flowrate is constant, as it is usually done in grinding setups, the best inlet boundary condition is the mass flowrate boundary condition, and is therefore used in this work, instead of pressure inlet.

### 2.4.6.14.3 Volume Fraction Specification

For the case of subcritical inlet flows, FLUENT software uses the values from the neighboring cells in order to reconstruct the volume fraction values on the boundary. That is done by using the following procedure [10]:

- First compute the node values of volume fraction at the boundary using the values in the cell.
• Second, compute the volume fraction at the every boundary face using the interpolated node values.

For the case of supercritical inlet flows the volume fraction value on the boundary can be computed by using the free surface fixed height.

2.4.6.15 Downstream Boundary Conditions

2.4.6.15.1 Pressure Outlet

The static pressure at the outlet was specified as the gauge pressure. In the case of subcritical outlet flows (Fr < 1), and if there are only two phases in the computational domain, the pressure is taken from the profile of pressure specified over the boundary. In other cases, the pressure is taken from the neighboring computational cell. If flow is supercritical (Fr > 1), the pressure is always taken from the neighboring computational cell.

2.4.6.15.2 Outflow Boundary

In order to model flow exits in cases when the details of the flow velocity and pressure are unknown before the flow problem solution, outflow boundary conditions can be used at the outlet boundary of open channel flows. If the conditions are not known at the
outflow boundaries, FLUENT software extrapolates the required information from the interior of the computational domain.

There are significant limitations of this boundary type [10]:

- Only one outflow boundaries can be used at the outlet, which is done by setting the flow rate weighting to 1; therefore, outflow splitting is not allowed in open channel flows with outflow boundaries
- An initial flow field should be specified in the simulation in order to avoid convergence problems that arise because of flow reversal at the outflow, which will result in an unreliable solution
- An outflow boundary condition is not compatible with pressure inlets and pressure outlets; therefore, it can only be used with mass flow inlets
- An important assumption of this boundary condition is that flow is fully developed in the direction that is perpendicular to the outflow boundary surface

Because outflow boundary condition does not correspond to physics of the flow encountered in the models presented in this work (there exist flow splitting at different outflow boundaries and there is no fully developed flow in direction perpendicular to the outflow boundary surface), and its limitations, pressure outlet boundary conditions are used.
2.4.7 Eulerian Model

In fluid flows in grinding, along with the compact streams of metalworking liquid, there exist liquid droplets which form a kind of mist [1]. VOF model is good for simulating flows in which interface length between two fluids is of significant fraction of the size of the computational domain. That may not be case if droplets are present in the domain, too. Therefore, the Eulerian model, which is good for droplet-based flows, is also used in simulations performed as a part of this work.

The Eulerian multiphase model is capable of modeling flows with multiple separate, mutually interacting phases. The model allows phases such as liquids, gases, or solids or almost any combination of phases. For each phase an Eulerian treatment is used, unlike the Eulerian-Lagrangian treatment which is used for the discrete phase model [10].

With this model, memory requirements and convergence behavior limit the number of secondary phases. Therefore, there is no restriction on number of secondary phases that can be included if sufficient computer memory is available. For cases in which very complex multiphase flows exist, the solution may be limited by convergence behavior.

The solution of Eulerian multiphase model in FLUENT software is based on the following [10]:

- A single pressure is shared by all phases
- Momentum and continuity equations are solved for each phase
- Several interphase functions for drag coefficient are available, which are adequate for various types of multiphase regimes
• All of the k-epsilon turbulence models are available, and may apply to all phases or to the mixture.

2.4.7.1 Volume Fractions

Multiphase flow, described as interpenetrating continua, includes the concept of so-called “phasic volume fractions”, \( \alpha_q \). Volume fractions stand for the space that each phase occupies. The conservation laws for mass and momentum are satisfied by every phase individually. In order to derive the conservation equations, ensemble averaging the local instantaneous balance for every phase can be done [31] or there is an option to use the mixture theory approach [32].

The volume of phase \( q \), \( V_q \), is defined by [10]:

\[
V_q = \int \alpha_q dV
\]

(2.32)

where \( \sum_{q=1}^{n} \alpha_q = 1 \).

The effective density of phase \( q \) is [10]:

\[
\hat{\rho}_q = \alpha_q \rho_q
\]

(2.33)

where \( \rho_q \) is the physical density of phase \( q \).

2.4.7.2 Conservation of Mass
The continuity equation for phase \( q \) is as follows [10]:

\[
\frac{\partial}{\partial t} (\alpha_q \cdot \rho_q) + \nabla \cdot (\alpha_q \cdot \rho_q \cdot \vec{v}_q) = \sum_{p=1}^{n} (\dot{m}_{pq} - \dot{m}_{qp}) + S_q ,
\]  

(2.34)

where:

- \( \vec{v}_q \) is the velocity of phase \( q \)
- \( \dot{m}_{pq} \) is the mass transfer from the \( p \)th to \( q \)th phase
- \( \dot{m}_{qp} \) is the mass transfer from phase \( q \) to phase \( p \).

The source term \( S_q \) on the right-hand side of Eq. (2.32) can be zero or can be specified as constant or variable mass source for every phase. There is a similar term that appears in the momentum and enthalpy equations.

### 2.4.7.3 Conservation of Momentum

The momentum balance for phase \( q \) yields [10]:

\[
\frac{\partial}{\partial t} (\alpha_q \cdot \rho_q \cdot \vec{v}_q) + \nabla \cdot (\alpha_q \cdot \rho_q \cdot \vec{v}_q) = -\alpha_q \cdot \nabla p + \nabla \cdot \vec{\tau}_q + \alpha_q \cdot \rho_q \cdot \vec{g} + \sum_{p=1}^{n} \left( \vec{R}_{pq} + \dot{m}_{pq} \cdot \vec{v}_q - \dot{m}_{qp} \cdot \vec{v}_q \right) + \left( \vec{F}_q + \vec{F}_{ijq} + \vec{F}_{vmq} \right) ,
\]  

(2.35)

where \( \vec{\tau}_q \) is the \( q \)th phase stress-strain tensor, computed as [10]:

\[
\vec{\tau}_q = \alpha_q \cdot \mu_q \cdot \left( \nabla \vec{v}_q + \nabla \vec{v}_q^T \right) + \alpha_q \cdot \left( \lambda_q - \frac{2}{3} \cdot \mu_q \right) \cdot \nabla \cdot \vec{v}_q \cdot \vec{I} .
\]  

(2.36)
Here:

- $\mu_q$ and $\lambda_q$ are the shear and bulk viscosity of phase $q$
- $\vec{F}_q$ is an external body force
- $\vec{F}_{lift,q}$ is a lift force
- $\vec{F}_{vm,q}$ is a virtual mass force
- $\vec{R}_{pq}$ is an interaction force between phases
- $p$ is the pressure shared by all phases
- $\vec{v}_{pq}$ is the interphase velocity, defined as: if $\dot{m}_{pq} > 0$ (i.e., phase $p$ mass is being transferred to phase $q$), $\vec{v}_{pq} = \vec{v}_p$; if $\dot{m}_{pq} < 0$ (i.e., phase $q$ mass is being transferred to phase $p$), $\vec{v}_{pq} = -\vec{v}_q$; similarly, if $\dot{m}_{qp} > 0$ then $\vec{v}_{qp} = \vec{v}_q$, if $\dot{m}_{qp} < 0$ then $\vec{v}_{qp} = -\vec{v}_p$.

Equation (2.35) must be closed with adequate expressions for the interphase force $\vec{R}_{pq}$. This interphase force is dependent on the friction, pressure, cohesion, and other effects. It is also subject to the conditions that $\vec{R}_{pq} = -\vec{R}_{qp}$ and $\vec{R}_{qq} = 0$[10].

A simple interaction term of the following form can be used for the interphase force [10]:

$$\sum_{p=1}^{n} \vec{R}_{pq} = \sum_{p=1}^{n} K_{pq} \cdot (\vec{v}_p - \vec{v}_q),$$

(2.37)

where $K_{pq} (= K_{qp})$ is the interphase momentum exchange coefficient.
2.4.7.4 Lift Forces

The effect of lift forces on the secondary phase droplets (or bubbles or particles) can be included in multiphase flows. The reason that these lift forces appear is mostly due to velocity gradients in the primary-phase flow field. For larger particles the lift force is more significant.

The lift force acting on a secondary phase \( p \) in a primary phase \( q \) is calculated as [33]:

\[
\vec{F}_{lift} = -0.5 \cdot \rho_q \cdot \alpha_p \cdot \left( \vec{v}_q - \vec{v}_p \right) \times \left( \nabla \times \vec{v}_q \right).
\] (2.38)

The lift force \( \vec{F}_{lift} \) is be added to the right-hand side of the momentum equation for both phases (\( \vec{F}_{lift,q} = -\vec{F}_{lift,p} \)) [10].

If the lift force is significant this term should be included. The model allows the lift force and lift coefficient to be specified for each pair of phases.

2.4.7.5 Virtual Mass Force

If a secondary phase \( p \) accelerates relative to the primary phase \( q \) the "virtual mass effect" is included. The inertia of the primary-phase mass encountered by the accelerating droplets (or bubbles or particles) exerts a "virtual mass force" on the droplets [33]:

\[
\vec{F}_{vm} = 0.5 \cdot \alpha_p \cdot \rho_q \cdot \left( \frac{d_q \vec{v}_q}{dt} - \frac{d_p \vec{v}_p}{dt} \right).
\] (2.39)
The term \( \frac{d_q}{dt} \) is the phase material time derivative that can be expressed as [10]:

\[
\frac{d_q(\phi)}{dt} = \frac{\partial(\phi)}{\partial t} + (\vec{v}_q \cdot \nabla)\phi. \tag{2.40}
\]

The virtual mass force \( \vec{F}_{vm} \) is added to the right-hand side of the momentum equation for both phases \( (\vec{F}_{vm,q} = -\vec{F}_{vm,p}) \) [10].

The virtual mass effect is significant when density of secondary phase is a lot smaller than the primary phase density.

2.4.7.6 Conservation of Energy

The conservation of energy in applications involving Eulerian multiphase model, can be described by writing a separate enthalpy equation for each phase [10]:

\[
\frac{\partial}{\partial t}(\alpha_q \cdot \rho_q \cdot h_q) + \nabla \cdot (\alpha_q \cdot \rho_q \cdot \vec{u}_q \cdot h_q) = -\alpha_q \cdot \frac{\partial p_q}{\partial t} + \tau_q + \nabla \vec{u}_q - \\
\nabla \cdot \vec{q}_q + S_q + \sum_{p=1}^{n}(Q_{pq} + \dot{m}_{pq} \cdot h_{pq} - \dot{m}_{qp} \cdot h_{qp}), \tag{2.41}
\]

where

- \( h_q \) is the specific enthalpy of the q\textsuperscript{th} phase
- \( \vec{q}_q \) is the heat flux
- \( S_q \) is a source term that includes sources of enthalpy
- \( Q_{pq} \) is the intensity of heat exchange between the p\textsuperscript{th} and q\textsuperscript{th} phases
• $h_{pq}$ is the interphase enthalpy

The heat exchange between phases has to comply with the local balance conditions $Q_{pq} = -Q_{qp}$ and $Q_{qq} = 0$ [10].

2.4.7.7 Interphase Exchange Coefficients

The momentum exchange between the phases is derived from the value of the fluid-fluid exchange coefficient $K_{pq}$.

For fluid-fluid flows, every secondary phase is assumed to form bubbles or droplets. This is important in assignment of each of the fluids a particular phase. In multiphase flows where exist unequal amounts of two fluids, the primary fluid should be the predominant fluid. That is because the less abundant fluid is more likely to form bubbles or droplets. The exchange coefficient for these types of multiphase flow can be expressed by the following general form [10]:

$$K_{pq} = \frac{\alpha_q \cdot \alpha_p \cdot \rho_p \cdot f}{\tau_p},$$

(2.42)

where

• $f$, the drag function, is defined differently for the different exchange-coefficient models

• $\tau_p$, the "particulate relaxation time", can be defined as: $\tau_p = \frac{\rho_p \cdot d_p^2}{18 \cdot \mu_q}$
• \( d_p \) is the diameter of the droplets or bubbles of phase p.

Basically, every definition of \( f \) includes a drag coefficient, \( C_D \), that is based on the relative Reynolds number. This drag function is different between the exchange-coefficient models. In all situations, \( K_{pq} \) tends to zero whenever the primary phase is not within a domain. In order to enforce this, the volume fraction of the primary phase \( q \) multiplies the drag function \( f \).

The usually used definitions of \( f \) are from work of Schiller and Naumann [34] and from work of Morsi and Alexander [35].

For the model of Schiller and Naumann [34]:

\[
f = \frac{C_D \cdot \text{Re}}{24},
\]

where

\[
C_D = \begin{cases} 
\frac{24 \cdot (1 + 0.15 \cdot \text{Re}^{0.687})}{\text{Re}}, & \text{Re} \leq 1000 \\
0.44, & \text{Re} > 1000 
\end{cases} 
\]

The relative Reynolds number, \( \text{Re} \) in Eq. (2.43) for the primary phase \( q \) and secondary phase \( p \) can be calculated as [34]:

\[
\text{Re} = \frac{\rho_q \cdot |\vec{v}_p - \vec{v}_q| \cdot d_p}{\mu_q}.
\]

The relative Reynolds number for secondary phases \( p \) and \( r \) can be calculated as [34]:

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In Eq. (2.46) \( \mu_{rp} \) is the mixture viscosity of the phases p and r. It is calculated as [34]:

\[
\mu_{rp} = \alpha_p \mu_p + \alpha_r \mu_r.
\]  

(2.47)

The Schiller and Naumann model is adequate for general use for any fluid-fluid pair of phase.

For the Morsi and Alexander model [35]:

\[
f = \frac{C_D \cdot \text{Re}}{24},
\]  

(2.48)

where:

\[
C_D = a_1 + \frac{a_2}{\text{Re}} + \frac{a_3}{\text{Re}^2}.
\]  

(2.49)

Reynolds number is defined by Eq. (2.45) or Eq. (2.46). Parameters \( a_1, a_2 \) and \( a_3 \) are defined as follows [35]:
The model of Morsi and Alexander is considered as the most complete. It adjusts the definition of function \( f \) frequently over a very broad range of Reynolds numbers. The bad side of the model is that calculations that incorporate it tend to be less stable compared to other models [10].

\[
a_1, a_2, a_3 = \begin{cases} 
0.24, 0; 0 < \text{Re} < 0.1 \\
3.69, 22.73, 0.0903; 0.1 < \text{Re} < 1 \\
1.222, 29.1667, -3.8889; 1 < \text{Re} < 10 \\
0.6167, 46.5, -116.67; 10 < \text{Re} < 100 \\
0.3644, 98.33, -2778; 100 < \text{Re} < 1000 \\
0.357, 148.62, -47500; 1000 < \text{Re} < 5000 \\
0.46, -490.546, 578700; 5000 < \text{Re} < 10000 \\
0.5191, -1662.5, 5416700; \text{Re} \geq 10000
\end{cases}
\] (2.50)

2.4.7.8 Description of Heat Transfer

The internal energy balance for phase \( q \), Eq. (2.41), contains phase enthalpy term, which is defined as [10]:

\[
H_q = \int c_{p,q} \, dT_q,
\] (2.51)

where \( c_{p,q} \) represents the specific heat of phase \( q \) at constant pressure.

The heat exchange coefficient has to be calculated, too. It is assumed that rate of energy transfer between phases is a function of the temperature difference [10]:

\[
Q_{pq} = h_{pq} \cdot (T_p - T_q).
\] (2.52)
here $h_{pq} (= h_{qp})$ represents the heat transfer coefficient between the $p^{th}$ phase and the $q^{th}$ phase. The heat transfer coefficient can be related to the Nusselt number of the $p^{th}$ phase, $Nu_p$, by equation [10]:

$$
  h_{pq} = \frac{6 \cdot \kappa_q \cdot \alpha_p \cdot \alpha_q \cdot Nu_p}{d_p^2}.
$$

(2.53)

Here $\kappa_q$ represents the thermal conductivity of the $q^{th}$ phase. The Nusselt number can usually be calculated based on some of several correlations that can be found in the literature. One of correlations for fluid-fluid multiphase flow is, for example, correlation of Ranz and Marshall [36, 37]:

$$
  Nu_p = 2.0 + 0.6 \cdot Re_p^{\frac{1}{2}} \cdot Pr^{\frac{1}{2}},
$$

(2.54)

where:

- $Re_p$ is the relative Reynolds number based on the diameter of the $p^{th}$ phase and the relative velocity $|\bar{u}_p - \bar{u}_q|$, 
- $Pr$ represents the Prandtl number of the $q^{th}$ phase, defined as: $Pr = \frac{c_p \cdot \mu_q}{\kappa_q}$.

Nusselt number $h_{pq}$ should go to zero if one of the phases is not present inside the domain. To make sure that the criterion is satisfied, $h_{pq}$ is multiplied by the volume fraction of the primary phase $q$ every time.
2.5 Turbulence modeling

2.5.1 Introduction on turbulence

One of the most important characteristics of turbulent flows is a fluctuating velocity field. Fluctuations of velocity mix different transported quantities like energy, momentum, and species concentration, and cause them to fluctuate, too. In flows with high Reynolds numbers these fluctuations can be of high frequency and small scale, it is too computationally expensive perform Direct Numerical Simulations in practical engineering calculations, or some types of scientific research. Therefore, the exact, instantaneous governing equations are time-averaged, ensemble-averaged, or manipulated in other ways in order to remove the small scales. That results in a modified set of equations that are cheaper to solve computationally. The modified set of equations includes additional unknown variables. Turbulence modeling is necessary in order to compute unknown variables in terms of known quantities.

2.5.1.1 Reynolds averaging

At present level of computer development, it is not practical in most cases to directly solve, including smallest scales of the motions, time-dependent Navier-Stokes equations for turbulent flows of high Reynolds number in complex geometries. To alleviate this problem, two methods are usually applied to make the Navier-Stokes equations easier to
solve. In these methods the small-scale turbulent fluctuations are be directly simulated. Reynolds averaging (which results in Reynolds averaged Navier-Stokes equations – RANS) and filtering are those methods. They add additional terms to the governing equations. These terms have to be modeled in order to achieve a closure of equations. In this work, turbulence models that rely on Reynolds averaging are employed to simulate turbulent flows.

The RANS set of equations governs the transport of the time-averaged flow quantities. The whole range of the turbulent scales is modeled by this approach. Therefore, that method significantly reduces the computational power needed, and is broadly used in engineering science and practice. The RANS equations can also be used to calculate time-dependent fluid flows that have externally imposed (for example, time-dependent boundary conditions or sources) or self-sustained (for example, vortex-shedding, flow instabilities) unsteadiness. The main principle of Reynolds averaging method is that the flow variables present in the exact, instantaneous Navier-Stokes equations are decomposed into two parts:

- The mean (time-averaged) component
- Fluctuating component.

For the components of velocity that method results in [10]:

\[ u_i = \bar{u}_i + u_i' \]  

(2.55)

Here, \( \bar{u}_i \) and \( u_i' \) are the mean and fluctuating velocity components.
The other quantities are similarly decomposed:

\[ \phi = \bar{\phi} + \phi'. \]  

(2.56)

Here, \( \phi \) represents a scalar quantity such as pressure, energy, or species concentration.

If the expressions of decomposed form for all flow variables are put into the exact, instantaneous continuity and momentum equations, and if the time-averaging is applied, the result is so-called time-averaged equations. In Cartesian tensor form (the overbar on the mean velocity, \( \bar{u} \), is dropped) those equations can be written as follows [10]:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho \cdot u_i) = 0
\]

(2.57)

\[
\frac{\partial}{\partial t} (\rho \cdot u_i) + \frac{\partial}{\partial x_j} (\rho \cdot u_i \cdot u_j) = -\frac{\partial p}{\partial x_i} \bar{u}_j + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right) \right] + \frac{\partial}{\partial x_j} \left( -\rho \cdot \bar{u}_i \cdot u_j \right).
\]

(2.58)

The name of these equations is Reynolds-averaged Navier-Stokes equations (RANS). The general form of RANS equations is the same as the form of instantaneous Navier-Stokes equations, but the velocities and other flow variables now represent or time-averaged values. The additional terms that come from inertial terms of the original Navier-Stokes equations, represent the effects of the turbulence on the mean flow. These terms are called Reynolds stresses, \(-\rho \cdot \bar{u}_i \cdot u_j\), and have to be modeled in order to close the momentum equation [10].
The appropriate modeling of RANS equations requires that the Reynolds stresses in momentum equation are modeled as well. A widely encountered technique uses the Boussinesq hypothesis in order to relate the Reynolds stresses to the mean velocity gradients [10]:

\[- \rho \cdot u_i \cdot u_j = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \left( \rho \cdot k + \mu_t \cdot \frac{\partial u_k}{\partial x_k} \right) \cdot \delta_{ij}.\]  

(2.59)

Turbulence models such as Spalart-Allmaras model, the k-ε models, and the k-ω models use the Boussinesq hypothesis. One of the advantages of this method is the relatively low computational resource needed to compute the turbulent viscosity, \( \mu_t \). Spalart-Allmaras turbulence model has just one additional transport equation (which represents turbulent viscosity) that has to be solved; k-ε and k-ω models, include two additional transport equations (for the turbulence kinetic energy, k, and either the turbulence dissipation rate, \( \epsilon \), or the specific dissipation rate, \( \omega \)) that need to be solved. In case of k-ε and k-ω, \( \mu_t \) is calculated as a function of k and \( \epsilon \). The greatest disadvantage of the Boussinesq hypothesis approach is that \( \mu_t \) is assumed to be an isotropic scalar quantity, which is not strictly true, and in some flow problems not true at all.

There exists an alternative approach, called Reynolds-stress model (RSM), that solves transport equations for every term in the Reynolds stress tensor. It requires an additional scale-determining equation (normally for \( \epsilon \)). The result is that five additional transport equations must be solved in 2-D flows and seven in 3-D [10].

In many fluid flow problems, models based on the Boussinesq hypothesis can perform in a satisfactory manner. Then, the additional computational expense associated with
Reynolds stress model is not justified. On the other hand, the Reynolds-stress model is clearly superior for flows in which the anisotropic effect of turbulence has a dominant influence on the mean flow. Examples of cases like these are highly swirling flows (as encountered in grinding, partly due to high-speed spinning wheel) and stress-driven secondary flows [10]. In this work, three turbulence models, that are particularly suited for solving flows with rotation, separation and recirculation, were applied in order to get accurate results, and study their influence on different fluid flow and heat transfer parameters. These models are Reynolds-stress, realizable k-ε and SST k-ω.

2.5.1.1 Types of turbulence models

2.5.1.1.1 Realizable k-ε model

The realizable k-ε model is a relatively modern turbulence model, proposed by Shih et al. [38]. It differs from the standard k-ε model in two important ways [10]:

- The realizable k-ε model includes a new formulation for the turbulent viscosity
- From an exact equation for the transport of the mean-square vorticity fluctuation a new transport equation for the dissipation rate, \( \varepsilon \), has been derived.

The term "realizable" indicates that this k-ε model satisfies a set of particular mathematical constraints on the Reynolds stresses, that is consistent with the physics of turbulent flows. The standard k-ε model and the RNG k-ε model are not realizable.
A direct advantage of the realizable k-ε model is that it is much better in accurately prediction of the spreading rate of both planar and round jets. Usually, it also provides significantly better results for flows involving rotation, boundary layers under strong adverse pressure gradients, separation, and recirculation [10].

The mathematics of the realizable k-ε model relies on combination of the Boussinesq relationship and the eddy viscosity definition that results in the following expression for the normal Reynolds stress in an incompressible strained mean flow [10]:

$$\overline{u^2} = \frac{2}{3} \cdot k - 2 \cdot \nu_t \cdot \frac{\partial U}{\partial x}.$$ (2.60)

Using Equation for kinematic turbulent viscosity, $\nu_t \equiv \frac{\mu_t}{\rho}$, the result is that the normal stress, $\overline{u^2}$, that is, by definition, a positive quantity, becomes negative, which means "non-realizable", if the strain is large enough to satisfy [10]:

$$\frac{k \cdot \frac{\partial U}{\partial x}}{\varepsilon} > \frac{1}{3 \cdot C_{\mu}} \approx 3.7.$$ (2.61)

In the same manner, the Schwarz inequality for shear stresses:

$$\overline{u_\alpha \cdot u_\beta} \leq \overline{u_\alpha^2} \cdot \overline{u_\beta^2} \quad \text{(no summation over } \alpha \text{ and } \beta),$$ (2.62)

can be violated in the cases when the mean strain rate is large enough. The most clear-cut way to ensure the realizability (that is, positive values of normal stresses and Schwarz inequality for shear stresses) is to make the constant parameter $C_{\mu}$ variable by making it sensitive to the mean flow (mean deformation) and the turbulence parameters (k, ε).
Works of many modelers, such as Reynolds, suggest variable $C_\mu$ [10]. That concept is backed up by experimental evidence [10]. For example, $C_\mu$ is calculated as about 0.09 in the inertial sublayer of equilibrium boundary layers, and about 0.05 in a strong homogeneous shear flow [10].

The realizable k-$\varepsilon$ model has shown considerable improvement over the standard k-$\varepsilon$ model in modeling flows that include strong streamline curvature, vortices, and rotation [10]. Initial studies have proved that the realizable k-$\varepsilon$ model results in the best performance compared to other k-epsilon model types for several cases of separated flows and flows with complex secondary flow features [10].

A typical problem encountered in the standard k-$\varepsilon$ model or other traditional k-$\varepsilon$ models is with the modeled equation for the $\varepsilon$ (dissipation rate). The so-called round-jet anomaly (the name comes from the finding that the calculation of spreading rate in planar jets is accurate enough, but the prediction of the spreading rate for axisymmetric jets is relatively bad, which is unexpected) comes largely due to the modeled $\varepsilon$ equation [10].

The realizable k-epsilon model was made in order to address the aforementioned deficiencies of traditional k-$\varepsilon$ models by including the following [10]:

- A new turbulent-viscosity formula that involves a variable $C_\mu$ originally proposed by Reynolds
- A new model equation for $\varepsilon$ that is based on the dynamic equation of the mean-square vorticity fluctuation.

A disadvantage of the realizable k-$\varepsilon$ model is in producing non-physical turbulent viscosities in flows when the computational domain includes both rotating and stationary
fluid zones. That happens because of the fact that the realizable k-ε model contains the effects of mean rotation in the definition of the turbulent viscosity. The behavior of extra rotation effect was observed in simulations with single rotating reference frame systems and showed superior results compared to the standard k-ε model. But, because of the nature of this modification, if applied to multiple reference frame systems some caution should be taken [10].

The modeled transport equations for k and ε in the realizable k-ε model are [10]:

\[
\frac{\partial}{\partial t} (\rho \cdot k) + \frac{\partial}{\partial x_j} (\rho \cdot k \cdot u_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \cdot \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \cdot \varepsilon - Y_m + S_k \quad , \quad (2.63)
\]

and

\[
\frac{\partial}{\partial t} (\rho \cdot \varepsilon) + \frac{\partial}{\partial x_j} (\rho \cdot \varepsilon \cdot u_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \cdot \frac{\partial \varepsilon}{\partial x_j} \right] + \rho \cdot C_1 \cdot S \cdot \varepsilon - \rho \cdot C_2 \cdot \frac{\varepsilon^2}{k + \sqrt{\nu \cdot \varepsilon}} + C_{1c} \cdot \varepsilon \cdot C_{3c} \cdot G_b + S_\varepsilon \quad , \quad (2.64)
\]

where:

\[
C_1 = \max \left[ 0.43, \frac{\eta}{\eta + 5} \right]
\]

\[
\eta = S \cdot \frac{k}{\varepsilon}
\]

\[
S = \sqrt{2 \cdot S_j \cdot S_j}
\]
In these equations:

- $G_k$ is the generation of turbulence kinetic energy due to the mean velocity gradients
- $G_b$ is the generation of turbulence kinetic energy due to buoyancy
- $Y_M$ represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate
- $C_2$ and $C_{1\varepsilon}$ are constants
- $\sigma_k$ and $\sigma_\varepsilon$ are the turbulent Prandtl numbers for $k$ and $\varepsilon$, respectively.
- $S_k$ and $S_\varepsilon$ are user-defined source terms.

The $k$ equation is the same as in the standard $k$-$\varepsilon$ model but the model constants are different. On the other hand, the $\varepsilon$ equation is substantially different from those in other $k$-$\varepsilon$ models. An important feature of this model is that the production term in the $\varepsilon$ equation (the second term on the right-hand side of the equation) does not contain the production of $k$, which means that it does not have the same term as the other $k$-$\varepsilon$ models. It is common opinion that the present form of the equation has better representation of the spectral energy transfer. Another positive feature is that the destruction term (the next to last term on the right-hand side of $\varepsilon$ equation) never results in a singularity. It is because its denominator can never become zero, even in cases when $k$ vanishes or becomes negative. This feature is a contrast to older $k$-$\varepsilon$ models which can have a singularity due to $k$ in the denominator.

The realizable $k$-$\varepsilon$ model has been validated for a many types of flows [38, 39], together with rotating homogeneous shear flows, free flows including jets and mixing
layers, channel and boundary layer flows, and separated flows [10]. The performance of
the model in all these cases has been found to be significantly better than that of the
classical k-epsilon model. Particularly important fact is that the realizable k-ε model
resolves the round-jet anomaly – the prediction of the spreading rate for axisymmetric
jets is as good as that for planar jets [10].

Similarly to other k-ε models, the turbulent viscosity is calculated as follows [10]:

\[
\mu_t = \rho \cdot C_\mu \cdot \frac{k^2}{\varepsilon}.
\]  \hspace{1cm} (2.65)

The \( C_\mu \), which is no longer constant is computed as follows [10]:

\[
C_\mu = \frac{1}{A_0 + A_S \cdot \frac{k \cdot U^*}{\varepsilon}},
\]  \hspace{1cm} (2.66)

where:

\[
U^* = \sqrt{S_{ij} \cdot S_{ij} + \tilde{\Omega}_{ij} \cdot \tilde{\Omega}_{ij}}
\]

\[
\tilde{\Omega}_{ij} = \Omega_{ij} - 2 \cdot \varepsilon_{ijk} \cdot \omega_k
\]

\[
\Omega_{ij} = \overline{\Omega_{ij}} - \varepsilon_{ijk} \cdot \omega_k
\]

The term \( \overline{\Omega_{ij}} \) is the mean rate-of-rotation tensor viewed in a rotating reference frame
with the angular velocity \( \omega_k \). The model constants \( A_0 \) and \( A_S \) are:

\[
A_0 = 4.04
\]

\[
A_S = \sqrt{6 \cdot \cos \phi},
\]  \hspace{1cm} (2.67)
where:

- \( \phi = \frac{1}{3} \cos^{-1}\left(\sqrt{6} \cdot W\right) \)
- \( W = \frac{S_{ij} \cdot S_{jk} \cdot S_{ki}}{S^3} \)
- \( \tilde{S} = \sqrt{S_y \cdot S_y} \)
- \( S_{ij} = \frac{1}{2} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \).

Parameter \( C_\mu \) is a function of:

- The mean strain and rotation rates
- The angular velocity of the system rotation
- The turbulence fields (\( k \) and \( \varepsilon \)).

\( C_\mu \) in Eq. (2.65) takes the standard value of 0.09 for an inertial sublayer in an equilibrium boundary layer [10].

The model constants \( C_2, \sigma_k, \) and \( \sigma_\varepsilon \) have been tuned in order to make sure that the model is good for certain flows. The model constants are [10]:

- \( C_{1\varepsilon} = 1.44 \)
- \( C_2=1.9 \)
- \( \sigma_k =1.0 \)
- \( \sigma_\varepsilon = 1.2. \)
The term $G_k$, that represents the production of turbulence kinetic energy, $k$, is modeled in the same manner as in the other k-$\varepsilon$ models. From the k- transport exact equation term $G_k$ can be defined as follows [10]:

$$G_k = -\rho \cdot \vec{u}_i \cdot \vec{u}_j \cdot \frac{\partial u_j}{\partial x_i}.$$  

(2.68)

In order to compute $G_k$ in a way consistent with the Boussinesq hypothesis the following equation can be used [10]:

$$G_k = \mu_t \cdot S^2,$$  

(2.69)

where $S$ is the modulus of the mean rate-of-strain tensor, defined as $S = \sqrt{2 \cdot S_{ij} \cdot S_{ij}}$.

When a model includes both non-zero gravity field and temperature gradient at the same time, the k-$\varepsilon$ models include the generation of $k$ due to buoyancy ($G_b$), and the analogous contribution to the production of $\varepsilon$.

The generation of turbulence due to buoyancy can be calculated as [10]:

$$G_b = \beta \cdot g_i \cdot \frac{\mu_t}{\Pr_t} \cdot \frac{\partial T}{\partial x_i},$$  

(2.70)

where:

- $\Pr_t$ is the turbulent Prandtl number for energy
- $g_i$ is the component of the gravitational vector in the $i^{th}$ direction.
For both the standard and realizable $k$-$\varepsilon$ turbulence models, the default value of $Pr_t$ is 0.85.

The coefficient of thermal expansion, $\beta$, is defined as:

$$\beta = -\frac{1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_p . \quad (2.72)$$

From the transport equations for $k$ is evident that turbulence kinetic energy tends to be amplified ($G_b > 0$) in cases of unstable stratification. For flows with stable stratification, buoyancy works to suppress the turbulence ($G_b < 0$) [10].

The buoyancy effects on the generation of $k$ are fairly well understood, but the effect on $\varepsilon$ is not so clear [10].

The constant $C_{3\varepsilon}$ determines the degree to which $\varepsilon$ is affected by the buoyancy. The constant is calculated according to the following equation [10]:

$$C_{3\varepsilon} = \tanh \left| \frac{v}{u} \right| , \quad (2.73)$$

where:

- $v$ is the component of the flow velocity parallel to the gravitational vector
- $u$ is the component of the flow velocity perpendicular to the gravitational vector.

Following this way, $C_{3\varepsilon}$ takes value of one for buoyant shear layers in which the main flow direction aligns with the direction of gravity vector. For cases of buoyant shear layers that are normal to the gravitational vector, $C_{3\varepsilon}$ becomes zero [10].
The modeling of turbulent heat transport is done using the concept of Reynolds' analogy to turbulent momentum transfer. The "modeled" energy equation is therefore given as following [10]:

\[
\frac{\partial}{\partial t} (\rho \cdot E) + \frac{\partial}{\partial x_i} \left[ u_i \cdot (\rho \cdot E + p) \right] = \frac{\partial}{\partial x_j} \left( k_{\text{eff}} \cdot \frac{\partial T}{\partial x_j} + u_i \cdot (\tau_{ij})_{\text{eff}} \right) + S_h ,
\]

where:

- \( E \) is the total energy
- \( k_{\text{eff}} \) is the effective thermal conductivity
- and \( (\tau_{ij})_{\text{eff}} \) is the deviatoric stress tensor, defined as:

\[
(\tau_{ij})_{\text{eff}} \equiv \mu_{\text{eff}} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) - \frac{2}{3} \cdot \mu_{\text{eff}} \left( \frac{\partial u_k}{\partial x_i} \cdot \delta_{ij} \right).
\]

The term that involves \( (\tau_{ij})_{\text{eff}} \) represents the heating which arises from viscous effects, and is always calculated in the density-based solvers. It can be enabled in the pressure-based solver, too, as done in this work.

For the both standard and realizable k-\( \varepsilon \) models, the effective thermal conductivity can be calculated as follows [10]:

\[
k_{\text{eff}} = k + \frac{c_p \cdot \mu_t}{\text{Pr}_t}
\]

(2.75)

where \( k \), in this case, is the thermal conductivity. The default value of the turbulent Prandtl number is 0.85 [10].
Turbulent mass transfer is treated in similar way. For the standard and realizable $k-\varepsilon$ models, the default turbulent Schmidt number (the ratio of momentum diffusivity and mass diffusivity) is 0.7 [10].

2.5.1.1.2 SST $k$-omega model

The shear-stress transport (SST) $k-\omega$ model was developed by Menter [40] in order to efficiently combine the robust and accurate formulation of the $k-\omega$ model in the region near walls with the free-stream independence of the $k-\varepsilon$ model in the far field [10]. To accomplish this, the $k-\varepsilon$ model is transformed into a $k-\omega$ formulation. The SST $k$-omega model is very similar to the standard $k-\omega$ turbulence model, but incorporates the following refinements [10]:

- First, blending function multiplies both the standard $k-\omega$ model and the transformed $k-\varepsilon$ model and then the models are added together; the blending function is designed to take value of one in the near-wall region - that activates the standard $k-\omega$ model, and to take value of zero away from the wall - that activates the transformed $k-\varepsilon$ model
- The SST model includes a damped cross-diffusion derivative term in the $\omega$ equation
- The definition of the eddy viscosity is modified to address the transport of the turbulent shear stress
- The modeling constants are different.
These refinements contribute to increased accuracy and reliability of the SST $k$-$\omega$ model in a wider class of fluid flows, such as adverse pressure gradient flows, airfoils, transonic shock waves, compared to the standard $k$-$\omega$ model. Another important change is the inclusion of a cross-diffusion term in the $\omega$ equation and a blending function to guarantee that the model equations perform appropriately in both the near-wall and far-field regions.

The SST $k$-$\omega$ model equations have a form similar to the standard $k$-$\omega$ model [40]:

$$\frac{\partial}{\partial t} (\rho \cdot k) + \frac{\partial}{\partial x_i} (\rho \cdot k \cdot u_i) = \frac{\partial}{\partial x_j} \left( \Gamma_k \cdot \frac{\partial k}{\partial x_j} \right) + \tilde{G}_k - Y_k + S_k$$

(2.76)

$$\frac{\partial}{\partial t} (\rho \cdot \omega) + \frac{\partial}{\partial x_i} (\rho \cdot \omega \cdot u_i) = \frac{\partial}{\partial x_j} \left( \Gamma_\omega \cdot \frac{\partial \omega}{\partial x_j} \right) + G_\omega - Y_\omega + D_\omega + S_\omega$$

(2.77)

where:

- $\tilde{G}_k$ represents the generation of turbulence kinetic energy due to mean velocity gradients
- $G_\omega$ represents the generation of $\omega$
- $\Gamma_k$ and $\Gamma_\omega$ represent the effective diffusivity of $k$ and $\omega$, respectively
- $Y_k$ and $Y_\omega$ represent the dissipation of $k$ and $\omega$ due to turbulence
- $D_\omega$ represents the cross-diffusion term
- $S_k$ and $S_\omega$ are user-defined source terms.
2.5.1.1.2.1 Modeling the Effective Diffusivity

The effective diffusivities for the SST $k$-$\omega$ model are defined as follows [10]

\[
\Gamma_k = \mu + \frac{\mu_t}{\sigma_k},
\]

(2.78)

\[
\Gamma_\omega = \mu + \frac{\mu_t}{\sigma_\omega},
\]

(2.79)

where $\sigma_k$ and $\sigma_\omega$ are the turbulent Prandtl numbers for $k$ and $\omega$, respectively. The eddy viscosity, $\mu_t$, is calculated as follows [10]:

\[
\mu_t = \frac{\rho \cdot k}{\omega} \cdot \frac{1}{\max \left\{ \frac{1}{\alpha^* \cdot a_1 \cdot \omega}, \frac{S \cdot F_2}{\alpha^*} \right\}},
\]

(2.80)

where:

- $S$ is the strain rate magnitude
- $\sigma_k = \frac{1}{F_1 + \frac{1 - F_1}{\sigma_{k,1} + \sigma_{k,2}}}
- \sigma_\omega = \frac{1}{F_1 + \frac{1 - F_1}{\sigma_{\omega,1} + \sigma_{\omega,2}}}
- \alpha^* = \alpha^* \cdot \left( \frac{0.024 + \frac{\rho \cdot k}{6 \cdot \mu \cdot \omega}}{1 + \frac{\rho \cdot k}{6 \cdot \mu \cdot \omega}} \right)

The blending functions, $F_1$ and $F_2$, are defined as follows [10]:
\[ F_1 = \tanh(\Phi_1^+) \]

\[ \Phi_1 = \min \left[ \max \left( \frac{\sqrt{k}}{0.09 \cdot \omega \cdot y}, \frac{500 \cdot \mu}{\rho \cdot y^2 \cdot \omega} \right), \frac{4 \cdot \rho \cdot k}{\sigma_{\omega,2} \cdot D_{\omega}^+ \cdot y^2} \right] \]

\[ D_{\omega}^+ = \max \left[ 2 \cdot \rho \cdot \frac{1}{\sigma_{\omega,2}} \cdot \frac{1}{\omega} \cdot \frac{\partial k}{\partial x_j} \cdot \frac{\partial \omega}{\partial x_j}, 10^{-10} \right] \]

\[ F_2 = \tanh(\Phi_2^+) \]

\[ \Phi_2 = \max \left[ 2 \cdot \frac{\sqrt{k}}{0.09 \cdot \omega \cdot y}, \frac{500 \cdot \mu}{\rho \cdot y^2 \cdot \omega} \right] \]

where \( y \) represents the distance to the next surface and \( D_{\omega}^+ \) is the positive portion of the cross-diffusion term.

2.5.1.1.2.2 Modeling the Turbulence Production – production of \( k \)

The term \( \tilde{G}_k \) is the production of turbulence kinetic energy. It is defined as follows [10]:

\[ \tilde{G}_k = \min(G_k, 10 \cdot \rho \cdot \beta^* \cdot k \cdot \omega) \quad (2.81) \]

2.5.1.1.2.3 Modeling the Turbulence Production - Production of \( \omega \)

The term \( G_\omega \) represents the production of \( \omega \) and is calculated as follows [10]:
\[ G_\omega = \frac{\alpha}{V_t} \cdot G_k. \]  \hspace{1cm} (2.81)

This formulation is different from the classical k-\omega model. The difference between the SST k-\omega and regular k-\omega model is also in the manner the term \( \alpha_\infty \) is evaluated. In the regular k-\omega model, \( \alpha_\infty \) has as a constant value of 0.52. In the SST k-\omega model, \( \alpha_\infty \) is calculated as follows [10]:

\[ \alpha_\infty = F_1 \cdot \alpha_{\infty,1} + (1 - F_1) \cdot \alpha_{\infty,2}, \]  \hspace{1cm} (2.82)

where:

- \( \alpha_{\infty,1} = \frac{\beta_{i,1}}{\beta^*_\infty} - \frac{\kappa^2}{\sigma_{\infty,1} \cdot \sqrt{\beta^*_\infty}} \)
- \( \alpha_{\infty,2} = \frac{\beta_{i,2}}{\beta^*_\infty} - \frac{\kappa^2}{\sigma_{\infty,2} \cdot \sqrt{\beta^*_\infty}} \)
- \( \kappa \) is 0.41.

2.5.1.1.2.4 Modeling the Turbulence Dissipation - Dissipation of k

The term \( Y_k \) is the dissipation of turbulence kinetic energy, \( k \), and is defined in a analogous manner as in the regular k-\omega model. The difference between the two models is in the way the term \( f_{\beta^*} \) is defined. For the SST k-\omega model, \( f_{\beta^*} \) is a constant whose value is equal to one. Therefore [10]:

\[ Y_k = \rho \cdot \beta^* \cdot k \cdot \omega. \]  \hspace{1cm} (2.83)
2.5.1.1.2.4 Modeling the Turbulence Dissipation - Dissipation of $\omega$

The term $Y_\omega$ represents the dissipation of $\omega$, and is defined in a analogous way as in the regular $k$-$\omega$ model. The two models differ in the manner the terms $\beta_i$ and $f_\beta$ are defined. For the SST $k$-omega model, $f_\beta$ has a constant value equal to one. Therefore [10]:

$$Y_k = \rho \cdot \beta \cdot \omega^2. \quad (2.84)$$

$\beta_i$ is not constant, but calculated as follows [10]:

$$\beta_i = F_i \cdot \beta_{i,1} + (1 - F_i) \cdot \beta_{i,2}. \quad (2.85)$$

2.5.1.1.2.5 Cross-Diffusion Modification

By blending the standard $k$-$\omega$ model and the standard $k$-$\omega$ model the SST $k$-omega model was formulated. In order to combine these two standard models together, the standard $k$-$\varepsilon$ model has been changed into equations based on $k$ and $\omega$. That procedure results in the introduction of a cross-diffusion term ($D_\omega$ in Eq. (2.77)). $D_\omega$ is calculated as follows [10]:

$$D_{\omega} = 2 \cdot (1 - F_i) \cdot \rho \cdot \sigma_{\omega,2} \cdot \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}. \quad (2.86)$$
The constants are as follows [10]:

\[
\begin{align*}
\sigma_{k,1} &= 1.176 \\
\sigma_{\omega,1} &= 2.0 \\
\sigma_{k,2} &= 1.0 \\
\sigma_{\omega,2} &= 1.168 \\
a_i &= 0.31 \\
\beta_{i,1} &= 0.075 \\
\beta_{i,2} &= 0.0828
\end{align*}
\]

All other model constants (\(\alpha_{\omega}^*, \alpha_{\omega}, \alpha_0, \beta_{\omega}^*, R_{\mu}, R_k, R_{\omega}, \zeta^*, \) and \(M^{i0}\)) have the same values as for the standard k-\(\omega\) model [10].

2.5.1.1.2 Wall Boundary Conditions

The boundary conditions for a wall in the \(k\) equation in the \(k-\omega\) models are treated in the same manner as the \(k\) equation is treated in case of enhanced wall treatment in the \(k-\epsilon\) models. Therefore, all boundary conditions for wall-function grids correspond to the wall function approach, while for the fine grids the adequate low-Reynolds-number boundary conditions is applied.

The value of \(\omega\) at the wall is defined as follows [10]:

\[
\omega_w = \frac{\rho \cdot (u^*)^2}{\mu} \cdot \omega^+
\]

(2.87)

The asymptotic value of \(\omega^+\) in the laminar sublayer is calculated as [10]:

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\[
\omega^+ = \min \left( \omega^+_w, \frac{6}{\beta_i \cdot (y^+)^2} \right)
\]

(2.88)

where:

- \( \omega^+_w = \begin{cases} 
(50/k_s^+)^2, & k_s^+ < 25 \\
100/k_s^+, & k_s^+ \geq 25 
\end{cases} \)

- \( k_s^+ = \max \left( 1.0, \frac{\rho \cdot k_s \cdot u^*}{\mu} \right) \)

- \( k_s \) is the roughness height.

In the logarithmic (or turbulent) region, the value of \( \omega^+ \) is [10]:

\[
\omega^+ = \frac{1}{\sqrt{\beta^+_{\text{turb}}}} \cdot \frac{du^+_\text{turb}}{dy^+}.
\]

(2.89)

From that, the value of \( \omega \) in the wall cell is computed as [10]:

\[
\omega = \frac{u^*}{\sqrt{\beta^+_{\text{turb}} \cdot \kappa \cdot y}}.
\]

(2.90)

If a wall cell is placed in the buffer region, \( \omega^+ \) is blended between the logarithmic and laminar sublayer values [10].
2.5.1.1.3 Reynolds stress model

The Reynolds stress model (RSM) is based on the work of Launder et al. [42,43,44] The model abandons the hypothesis of isotropic eddy-viscosity and closes the RANS equations by method of solving transport equations for the Reynolds stresses and an equation for the dissipation rate. That results in five additional transport equations that are required to be solved in 2-D flows and seven additional transport equations in 3-D flows.

Given that the RSM turbulence model includes effects of streamline curvature, swirl, rotation, and rapid changes in strain rate in a more precise way compared to one-equation and two-equation models, it has higher potential to accurately solve complex flows. The On the other hand, RSM predictions are still limited by the closure assumptions used to model different terms in the exact transport equations for the Reynolds stresses. A particular problem is the modeling of the pressure-strain and dissipation-rate terms, and usually thought to be responsible for compromising the accuracy of RSM computations [10].

The RSM model is more computationally expensive compared to two-equation models such as k-ε and k-ω and other simpler models. Therefore, sometimes it is not justifiable to use it if gains are not significant enough. Nevertheless, use of the RSM is considered a must if the flow features of interest result from anisotropy in the Reynolds stresses. Some of the examples are cyclone flows, highly swirling flows in combustors, rotating flow passages, and the stress-induced secondary flows in ducts [10].
In order to obtain the exact form of the Reynolds stress transport equations, moments of the exact momentum equation are taken. In this process a fluctuating property multiplies the exact momentum equations. The resulting product is then Reynolds-averaged. Several terms in the exact equation are not known. Therefore, it is required to make modeling assumptions in order to close the equations [10].

The exact transport equations for the transport of the Reynolds stresses, \( \rho \cdot \overline{u_i \cdot u_j} \), is as follows [10]:

\[
\frac{d}{dt} \left( \rho \cdot \overline{u_i \cdot u_j} \right) + \frac{\partial}{\partial x_k} \left( \rho \cdot \overline{u_k \cdot u_i \cdot u_j} \right) = - \frac{\partial}{\partial x_k} \left( \rho \cdot \overline{u_i \cdot u_j \cdot u_k} + p \cdot (\delta_{ij} \cdot u_i + \delta_{ij} \cdot u_j) \right) + \frac{\partial}{\partial x_k} \left[ \mu \cdot \frac{\partial}{\partial x_k} \left( \overline{u_i \cdot u_j} \right) \right]
- \rho \cdot \left( \overline{u_i \cdot u_k} \cdot \frac{\partial u_j}{\partial x_k} \right) + \rho \cdot \beta \cdot \left( \overline{u_i \cdot u_j \cdot \theta} + \overline{u_j \cdot u_i \cdot \theta} \right) + \rho \cdot \left( \overline{\partial u_i}{\partial x_j} + \overline{\partial u_j}{\partial x_i} \right) - 2 \cdot \mu \cdot \frac{\partial u_j}{\partial x_k} \frac{\partial u_j}{\partial x_k}
+ 2 \cdot \rho \cdot \Omega_k \cdot \left( \overline{u_j \cdot u_m \cdot \varepsilon_{jm} + u_j \cdot u_m \cdot \varepsilon_{jm}} \right) + S_{user} .
\] (2.91)

Terms in Eq. (2.91) are:

- \( \frac{d}{dt} \left( \rho \cdot \overline{u_i \cdot u_j} \right) \) is local time derivative

- \( \frac{\partial}{\partial x_k} \left( \rho \cdot \overline{u_k \cdot u_i \cdot u_j} \right) = C_{ij} \) is convection term

- \( - \frac{\partial}{\partial x_k} \left[ \rho \cdot \overline{u_i \cdot u_j \cdot u_k} + p \cdot (\delta_{ij} \cdot u_i + \delta_{ij} \cdot u_j) \right] = D_{T,ij} \) is turbulent diffusion term

- \( \frac{\partial}{\partial x_k} \left[ \mu \cdot \frac{\partial}{\partial x_k} \left( \overline{u_i \cdot u_j} \right) \right] = D_{L,ij} \) is laminar diffusion term

- \( - \rho \cdot \left( \overline{u_i \cdot u_k} \cdot \frac{\partial u_j}{\partial x_k} + \overline{u_j \cdot u_k} \cdot \frac{\partial u_i}{\partial x_k} \right) = P_{ij} \) is stress production term
• \(-\rho \cdot \beta \left( g_i \cdot \overline{u_j} \cdot \theta + g_j \cdot \overline{u_i} \cdot \theta \right) = G_{ij}\) is buoyancy production term

• \(p \left( \frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right) = \varphi_{ij}\) is pressure strain term

• \(2 \cdot \mu \frac{\partial \overline{u_i}}{\partial x_k} \frac{\partial \overline{u_j}}{\partial x_k} = \varepsilon_{ij}\) is dissipation term

• \(-2 \cdot \rho \cdot \Omega_k \left( \overline{u_j} \cdot \overline{u_m} \cdot \varepsilon_{ikm} + \overline{u_i} \cdot \overline{u_m} \cdot \varepsilon_{jm} \right) = F_{ij}\) is production by system rotation term

• \(S_{user}\) is user-defined source term.

Terms \(C_{ij}, D_{L,ij}, P_{ij},\) and \(F_{ij}\) do not require modeling. On the other hand, \(D_{T,ij}, G_{ij}, \varphi_{ij},\) and \(\varepsilon_{ij}\) need to be modeled in order to close the equations.

2.5.1.1.3.1 Modeling Turbulent Diffusive Transport

The modeling of term \(D_{T,ij}\) is often based on the generalized gradient-diffusion model of Daly and Harlow [45]:

\[
D_{T,ij} = C_s \frac{\partial}{\partial x_k} \left( \rho \frac{k \cdot \overline{u_k} \cdot \overline{u_i}}{\varepsilon} \frac{\partial \overline{u_i} \cdot \overline{u_j}}{\partial x_j} \right) .
\]

(2.92)

Using this, model equation can sometimes result in numerical instabilities. To alleviate that problem, a simplification with a scalar turbulent diffusivity can be used, as follows [46]:

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The eddy viscosity, \( \mu_t \), is computed as follows [10]:

\[
\mu_t = \rho \cdot C_\mu \cdot \frac{k^2}{\varepsilon},
\]

where constant \( C_\mu \) equals 0.09.

In work of Lien and Leschziner [47] a value of \( \sigma_k \) is specified as 0.82. That value is obtained by applying the Eq. (2.92) to a planar homogeneous shear flow.

2.5.1.1.3 Modeling the Pressure-Strain Term: Low-Re Stress-\( \omega \) Model

This model is a kind of a stress-transport model which is based on the \( \omega \) equations and LRR model [48]. The low-Re stress-\( \omega \) model is perfect for modeling fluid flows over curved surfaces and swirling flows, such as encountered in grinding applications.

The model resembles the k-\( \omega \) model because of its excellent accuracy when applied for a wide range of turbulent flows. In addition, modifications for low Reynolds number and rough surface boundary conditions are similar to the k-\( \omega \) model [10]. The equation for pressure-strain term with exclusion of wall reflections can be written for the low-Re stress-omega model as follows [10]:

\[
\phi_j = \phi_{j,1} + \phi_{j,2}.
\]
Therefore [10]:

\[
\phi \equiv -C_i \cdot \rho \cdot \beta^*_RSM \cdot \omega \cdot \left[ \frac{1}{3} \cdot \frac{2}{3} \cdot \delta \cdot \hat{k} \cdot \hat{k} \cdot \hat{\omega} \cdot \left( P_{ij} - \frac{1}{3} \cdot P_{kk} \cdot \delta \right) \right] - \\
\hat{\beta}_o \cdot \left[ D_{ij} - \frac{1}{3} \cdot P_{kk} \cdot \delta \right] - k \cdot \hat{\gamma}_0 \cdot \left[ S_{ij} - \frac{1}{3} \cdot S_{kk} \cdot \delta \right],
\]

(2.96)

where term \( D_{ij} \) is defined as follows [10]:

\[
D_{ij} = -\rho \cdot \left[ \frac{1}{3} \cdot \frac{2}{3} \cdot \delta \cdot \hat{k} \cdot \hat{k} \cdot \hat{\omega} \cdot \left( u_i \cdot u_j + u_j \cdot u_i \right) \cdot \frac{\partial u_m}{\partial x_i} \right],
\]

(2.97)

Term \( S_{ij} \) is the mean strain rate, and is defined as follows [10]:

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right).
\]

(2.98)

Term \( \beta^*_RSM \) can be defined as follows [10]:

\[
\beta^*_RSM = \beta^* \cdot f_{\beta^*},
\]

(2.99)

where \( \beta^* \) and \( f_{\beta^*} \) are defined as:

\begin{itemize}
  \item \( f_{\beta^*} = \begin{cases} 
    1, & \chi_k \leq 0 \\
    \frac{1 + 640 \cdot \chi_k^2}{1 + 400 \cdot \chi_k^2}, & \chi_k > 0,
  \end{cases} \) where \( \chi_k = \frac{1}{\omega^3} \cdot \frac{\partial k}{\partial x_j} \cdot \frac{\partial \omega}{\partial x_j} \)
  \item \( \beta^* = 0.09. \)
\end{itemize}
The constants are:

\[
\hat{\alpha}_0 = \frac{8 + C_2}{11}, \\
\hat{\beta}_0 = \frac{8 \cdot C_2 - 2}{11}, \\
\hat{\gamma}_0 = \frac{60 \cdot C_2 - 4}{55}, \\
C_1 = 1.8, \\
C_2 = 0.52
\]

The treatment of the low-Re stress-omega equation wall boundary conditions in Reynolds-stress models is in the same manner as for the k equation in the k-\(\omega\) models [10].

FLUENT defines the value of omega at the wall as

\[
\omega_w = \frac{\rho \cdot (u^*)^2}{\mu} \cdot \omega^+, \tag{2.100}
\]

where \(\omega^+\) is dimensionless quantity and is defined as follows [10]:

\[
\omega^+_w = \begin{cases} 
\left( \frac{50}{k_s^+} \right)^2, & k_s^+ < 25 \\
500, & k_s^+, k_r^+ \geq 25
\end{cases}
\]

where:

\[
k_s^+ = \frac{\rho \cdot k_s \cdot u^*}{\mu} \quad \text{is the roughness height.}
\]

The production terms due to buoyancy are modeled as [10]:

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\[ G_y = \beta \cdot \frac{\mu_t}{Pr} \left( g_i \cdot \frac{\partial T}{\partial x_j} + g_j \cdot \frac{\partial T}{\partial x_i} \right), \]  

(2.101)

where \( Pr_t = 0.85 \) is the turbulent Prandtl number for energy.

For ideal gases, \( G_y \) can be defined as follows [10]:

\[ G_y = -\frac{\mu_t}{\rho \cdot Pr} \left( g_i \cdot \frac{\partial \rho}{\partial x_j} + g_j \cdot \frac{\partial \rho}{\partial x_i} \right). \]  

(2.102)

2.5.1.1.3 Modeling the Turbulence Kinetic Energy

The turbulence kinetic energy can be obtained by method of taking the trace of the Reynolds stress tensor [10]:

\[ k = \frac{1}{2} u_i \cdot u_i. \]  

(2.103)

in order to obtain boundary conditions for the Reynolds stresses it is usual to solve a transport equation for the turbulence kinetic energy, \( k \).

The resulting equation is as follows [10]:

\[ \frac{\partial}{\partial t} (\rho \cdot k) + \frac{\partial}{\partial x_i} (\rho \cdot k \cdot u_i) = \frac{\partial}{\partial x_j} \left( \left( \mu + \frac{\mu_t}{\sigma_k} \right) \cdot \frac{\partial k}{\partial x_j} \right) + \]

\[ \frac{1}{2} \left( P_{ii} + G_{ii} \right) - \rho \cdot \varepsilon \left( 1 + 2 \cdot M_i^2 \right) + S_k, \]  

(2.104)
where:

- $\sigma_k = 0.82$
- $S_k$ is a user-defined source term.

Even though Eq. (2.104) is solved globally all over the flow domain, the obtained values of $k$ are used just for the boundary conditions. For all other cases, $k$ is calculated using Eq. (2.103).

### 2.5.1.1.3.4 Modeling the Dissipation Rate

The dissipation tensor, $\varepsilon_{ij}$, is modeled as follows [10]:

$$
\varepsilon_{ij} = \frac{2}{3} \cdot \delta_{ij} \cdot \left( \rho \cdot \varepsilon + Y_M \right).
$$

(2.105)

Here, $Y_M = 2 \cdot \rho \cdot \varepsilon \cdot M_t^2$ is an extra "dilatation dissipation" term which comes from the work of Sarkar [49]. The turbulent Mach number used in this term is defined as follows [10]:

$$
M_t = \frac{k}{\sqrt{a^2}}.
$$

(2.106)

Here, $a = \sqrt{\gamma \cdot R \cdot T}$ is the speed of sound. This compressibility modification always takes effect only if the compressible form of the ideal gas law is applied.

A model transport equation is used to calculate the scalar dissipation rate, $\varepsilon$, as follows [10]:

$$
\frac{\partial k}{\partial t} + \nabla \cdot (\vec{u} k) = \nabla \cdot \left( \frac{\mu_k}{\sigma_k} \theta \nabla k \right) + S_k - \rho \varepsilon.
$$

(2.107)
\[
\frac{\partial}{\partial t} (\rho \cdot e) + \frac{\partial}{\partial x_j} (\rho \cdot e \cdot u_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_e} \right) \cdot \frac{\partial e}{\partial x_j} \right] \cdot C_{e1} \cdot \frac{1}{2} \left[ P_{ij} + C_{e3} \cdot G_{ij} \right] \cdot \frac{e}{k} \\
- C_{e2} \cdot \rho \cdot \frac{e^2}{k} + S_e
\]

, (2.107)

where:

- \( \sigma_e = 1.0 \)
- \( C_{e1} = 1.44 \)
- \( C_{e2} = 1.92 \)
- \( C_{e3} \) is evaluated as a function of the local flow direction relative to the gravitational vector
- \( S_e \) is a user-defined source term.

2.5.1.1.3.5 Wall Boundary Conditions

In Reynolds-stress model boundary conditions for each Reynolds stress, \( \overline{u_i \cdot u_j} \), and for the turbulence dissipation rate, \( \varepsilon \) (or \( \omega \) if the low-Re stress-omega model is used) are required [10]. In simulations performed in this work, these quantities are derived from the turbulence intensity and characteristic length, as described in Eqs. (2.4) and (2.5).

The near-wall values of the Reynolds stresses and \( \varepsilon \) are computed from wall functions [10]. The explicit wall boundary conditions for the Reynolds stresses are applied by using the logarithm law and the assumption of equilibrium. Convection and diffusion in the transport equations for the stresses are disregarded [10]. In order to calculate the
Reynolds stresses at the wall-adjacent cells (assuming standard wall functions or non-equilibrium wall functions) a local coordinate system is used, where:

- \( \tau \) is the tangential coordinate
- \( \eta \) is the normal coordinate
- \( \lambda \) is the binormal coordinate.

The result is:

\[
\frac{\overline{u_x^2}}{k} = 1.098, \quad \frac{\overline{u_y^2}}{k} = 0.247, \quad \frac{\overline{u_z^2}}{k} = 0.655, \quad -\frac{\overline{u_x u_y}}{k} = 0.255.
\]

Calculation of \( k \) is performed by solving the transport equation of Eq. (2.104). It is computationally convenient to solve the equation globally, despite the fact that the values of \( k \) computed in that manner are needed only close to the wall. For the region of the far field, turbulence kinetic energy, \( k \), is calculated directly from the normal Reynolds stresses using Eq. (2.103). The values of the Reynolds stresses close to the wall have a fixed value as described already. The transport Eqs. (2.91) are solved just in the region of the bulk flow.

Another approach is to specify the Reynolds stresses explicitly in terms of wall-shear stress, instead of turbulent kinetic energy.

Then, the result is [10]:

\[
\frac{\overline{u_x^2}}{u_x^2} = 5.1, \quad \frac{\overline{u_y^2}}{u_x^2} = 1.0, \quad \frac{\overline{u_z^2}}{u_x^2} = 2.3, \quad -\frac{\overline{u_x u_y}}{u_x^2} = 1.0.
\]

Here, \( u_x \) is so-called “friction velocity” defined by: \( u_x \equiv \sqrt{\frac{\tau_w}{\rho}} \), where \( \tau_w \) is the wall-shear stress.
2.5.1.1.3.6 Convective Heat and Mass Transfer Modeling

Reynolds' analogy to turbulent momentum transfer concept is usually used to model the turbulent heat transport in RSM. The energy equation is given as follows [10]:

$$\frac{\partial}{\partial t} (\rho \cdot E) + \frac{\partial}{\partial x_i} [u_i \cdot (\rho \cdot E + p)] = \frac{\partial}{\partial x_j} \left[ \left( k + \frac{c_p \cdot \mu_i}{\Pr} \right) \frac{\partial T}{\partial x_j} + u_i \cdot \tau_{ij}^\text{eff} \right] + S_h$$

(2.108)

where:

- $E$ is the total energy
- $(\tau_{ij})^\text{eff}$ is the deviatoric stress tensor: $(\tau_{ij})^\text{eff} \equiv \mu^\text{eff} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu^\text{eff} \frac{\partial u_k}{\partial x_k} \delta_{ij}$.

The term that involves $(\tau_{ij})^\text{eff}$ is the effect of the viscous heating. It is always calculated in the density-based solvers, and can be enabled in the pressure-based solver, as done in simulations performed in this work. The turbulent Prandtl number has a default value of 0.85.

A similar treatment is applied to the turbulent mass transfer, with a default value of 0.7 for turbulent Schmidt number.

2.6 Boundary conditions

Boundary conditions are a set of restraints, applied to governing equations, which specify the flow and thermal variables at the boundaries of a computational model. They
are considered to be of a critical importance for accuracy and stability of any CFD simulation. Therefore, boundary value problems must be well-posed. That means that the mathematical models of physical phenomena applied in the problem have to satisfy certain criteria [50]:

- A solution of the problem must exist
- The solution must be unique
- The solution is a continuous function of data, in some reasonable topology.

The boundary condition types used in this work can be classified as follows:

- Flow inlet boundaries: velocity inlet or mass flow inlet
- Flow exit boundaries: pressure outlets
- Wall boundary conditions: wall and symmetry
- Internal cell zones: fluid, and solid (porous is a type of fluid zone).
- Internal face boundaries: interior.

The further explanation of boundary conditions used in created models is in the following section.

2.6.1 Mass flow inlet boundary condition

The mass flow boundary condition provides a prescribed mass flow rate. This boundary condition is usually used when it is more important to match a prescribed mass
flow rate than to match the total pressure of the inflow stream. In grinding applications, the nozzle flowrate of metalworking fluid is specified as mass or volume flowrate.

2.6.2 Pressure outlet boundary condition

This type of a boundary condition requires the specification of a value for static (gauge) pressure at the outlet boundary. The remaining flow quantities are extrapolated from the interior. It is also required to specify a set of "backflow" conditions if the flow reverses direction at the pressure outlet boundary during the calculation process. There are several recommendations to minimize convergence difficulties [10]:

- If known, realistic values for the backflow quantities should be specified
- Lowering the under-relaxation factor from the default value
- It is desirable to place a limit for the pressure values in the zone by setting the minimum or maximum pressure values.

This strategy is frequently quite successful for many complex fluid flow problems.

2.6.3 Wall boundary condition

The default option in simulations of viscous flows is the no-slip boundary condition that is enforced at walls. No-slip boundary condition implies that the fluid moves with the same velocity as the wall. Based on the flow parameters in the local flow field, the computation of shear stress and heat transfer between the fluid and wall is performed. In
cases when heat transfer is included in the computational model, the energy equation has being solved. Therefore, thermal boundary conditions at walls have to be specified.

Some of the typical types of these boundary conditions are as follows [10]:

- Fixed heat flux
- Fixed temperature
- Convective heat transfer
- External radiation heat transfer
- Combined external radiation and convection heat transfer
- Heat generation.

In models built in this work, heat generation and fixed heat flux boundary conditions were used, at appropriate walls. According to the motion classification, wall boundaries are:

- Stationary – specifies a fixed wall
- Moving – translational or rotational velocity can be specified.

Walls can be specified as smooth or rough. The roughness affects flow resistance and heat and mass transfer on the walls. If a wall roughness is specified, computational model includes the law-of-the-wall modified for roughness [10]. In this work, grinding wheel is specified as a rough wall, with roughness value that corresponds to the selected grain size.
The equation of calculating heat transfer to the wall boundary from a solid cell is as follows [10]:

\[
q = \frac{k_s}{\Delta n} \cdot (T_w - T_s).
\]  

(2.109)

2.6.4 Fluid conditions

All active equations are solved for a group of computational cells called “a fluid zone”. FLUENT software requires the type of fluid material to be specified for a fluid zone in order to use appropriate material properties. Available inputs to the fluid zone are as follows [10]:

- Sources or fixed values of mass, momentum, heat (temperature), turbulence, species, and other scalar quantities.
- Motion for the fluid zone can be defined (as done in this work by setting the porous grinding region as moving)
- The rotation axis has to be specified for rotating zones (it was defined for the porous grinding region in this work).

2.6.5 Solid conditions

This condition is used for a group of cells for which just the heat conduction equation is solved. FLUENT software requirement is that the type of solid material has to be
provided in order to use the appropriate material properties. Inputs that are available are as follows [10]:

- Volumetric heat generation rates or a fixed value of temperature
- Solid zone motion (included in some of the simulations performed in this work)
- If there are rotationally periodic boundaries adjacent to the solid zone, the rotation axis has to be specified.

2.7 Numerical validation

In this work, three types of numerical validations were performed:

- Grid dependence study
- Mass imbalance check
- Numerical residual convergence criterion check.

When a CFD problem is solved, the solution should not be affected by the size of used grid. Therefore, grid independence study is done to ensure that the solution does not change significantly if the grid is refined.

The continuity equation has to be satisfied, too. In reality, mass cannot be destroyed or created out of nothing. Therefore, if incompressible solver is used, accounting for the different phases in a cell, the total mass flux should be equal to zero. But, because of the existence of numerical errors, a mass imbalance occurs. The objective is to minimize it,
and the simulation results should attain mass imbalance result which is below accepted levels.

The third numerical validation is concerned with numerical residuals which should fall to zero in a steady state computations. Because of the numerical errors or inherent unsteadiness of the flow, that cannot be true. Therefore, a set of limits is determined, based on the types of the solver used, flow in question and other parameters. When numerical residuals of different flow quantities fall below those limit values, the solution is said to be converged.

Hypothetically, if a simulation is run on a computer that has infinite precision, numerical residuals would go to zero as the solution converges. In reality, as simulation runs, the residuals decrease to some small value (so-called "round-off") and then they stop changing ("level out") [10]. In cases of single-precision computations, residuals can reduce in value as many as six orders of magnitude before they reach round-off. If computations are performed with double-precision computers, residuals can drop up to twelve orders of magnitude [10].

Discretized form of the conservation equation for a general variable \( \Phi \) at a cell \( P \) is as follows [10]:

\[
\mathbf{a}_p \cdot \Phi_p = \sum_{nb} a_{nb} \Phi_{nb} + b ,
\]

where:

- \( \mathbf{a}_p \) is the center coefficient defined as: \( a_p = \sum_{nb} a_{nb} - S_p \)
• $a_{nb}$ are the influence coefficients for the neighboring cells

• and $b$ is the contribution of two quantities: the constant part of the source term $S_c$ in $S = S_c + S_P \cdot \Phi$ and of the boundary conditions.

The described method scales the residual employing a scaling factor representative of the flow rate of $\Phi$ through the domain. The scaled residual is defined as [10]:

$$
R^\Phi = \frac{\sum_{\text{cells}_{-}P} \sum_{nb} a_{nb} \cdot \Phi_{nb} + b - a_P \cdot \Phi_p}{\sum_{\text{cells}_{-}P} |a_P \cdot \Phi_p|}.
$$

(2.111)

In the case of the momentum equations the term in the denominator, $a_P \cdot \Phi_p$, is replaced by term $a_P \cdot v_{p\_cell}$, where $v_{p\_cell}$ is the magnitude of the velocity at cell $P$. The scaled residual quantity is a more adequate indicator of convergence for most fluid flow problems [10]. In the case of the continuity equation, the unscaled residual for the pressure-based solver can be defined as [10]:

$$
R^c = \sum_{\text{cells}_{-}P} |\text{rate}\_\text{of}\_\text{mass}\_\text{creation}\_\text{in}\_\text{cell}\_P|.
$$

(2.112)

The scaled residual for the continuity equation in pressure-based solver can be defined as follows [10]:

$$
\frac{R^c_{\text{iteration}\_N}}{R^c_{\text{iteration}\_5}}.
$$

(2.113)

The denominator of Eq. (2.113) represents the largest absolute value of the continuity residual from the first five iterations.
There are no universally accepted metric for judging convergence. Residual limit values that are appropriate for one class of fluid flow problems can sometimes be deceptive for other classes of problems. For that reason a good idea is to judge convergence not just by examining residual values, but also by keeping an eye on important integrated flow quantities such as lift, drag or heat transfer coefficient. For most CFD problems, the convergence criterion set by default in FLUENT software is sufficient [10]. The criterion requires that the scaled residuals fall below $10^{-3}$ for all governing equations except the energy equation, for which the criterion is somewhat more demanding and is equal to $10^{-6}$. In some cases, however, this residual criterion can be inappropriate. If a good initial condition of the flow field is set, the starting continuity residual can be quite small. That leads to a large scaled residual for the continuity equation. In cases like that, a recommendation is to investigate the unscaled residual which should be compared with an appropriate scale like the inlet mass flowrate. For some quantities, such as encountered in turbulence, a bad initial condition can result in high scale factors. Then, scaled residuals will start with a low value and amplify as non-linear sources increase, and, at the end, decrease. Consequently, an appropriate method is to judge convergence not only from the value of the residual itself, but from its behavior. It should be checked that the residual values continue to fall, or remain small, for some number iterations (about 50 or more) before conclusion of solution convergence is made [10]. A different commonly used approach for convergence judging is a criterion that requires that the unscaled residuals fall by three orders of magnitude. In simulations performed the convergence criterion was that the scaled residuals should drop below recommended values.
Chapter Three

Description of numerical models and simulation results

3.1 3D Model 1

As a first step towards building a complete numerical model of the process fluid flow in grinding, the 3-D Model 1 simulates the global flow from the nozzle to the contact zone and out of the domain. The results of the simulations are used to evaluate the most important boundary conditions for the 3-D Model 2 that comprehensively simulates flow in the grinding region. The CFD model run in FLUENT software computes the solution of the Navier-Stokes equations with the appropriate boundary conditions.

Our results indicate that full 3D simulations of the flow over the wheel can be realistically obtained using current multi core computer workstations.
The 3-D Model 1 was used for two purposes:

- Understanding the global flow around the wheel and the grinding zone
- Generating the detailed boundary conditions for the 3-D Model 2.

3.1.1 Geometry

The computational domain contains solid surfaces, outflow boundary conditions and mass flowrate inlet. The solid surfaces in question are: shield, workpiece and grinding wheel. Between the wheel and the workpiece a 5 mm gap exists. The wheel diameter was 340 mm, and width was 50 mm. Figures 3-1 to 3-4 show the 3-D Model 1 geometry and its components.

![3-D Model 1 Geometry](image)

Figure 3-1: Solid Wall Boundaries in 3-D Model 1.
Figure 3-2: 3-D model 1 Solid Walls and Outflow Surfaces.

Figure 3-3: 3-D Model 1 Wireframe View.
Figure 3-4: 3-D model 1 Wireframe View.

3.1.2 Grid properties

The unstructured grid was created by using tetrahedral elements. Table 3.1 shows the most important grid quality parameters. The cell squish and cell skewness describe the cell deviation from the ideal shape. For that reason, the worst cells will have a cell squish and cell skewness close to 1. For most applications, the values should be below 0.9 [10]. Aspect ratio is a measure of cell stretching, and it is recommended that it does not exceed value of 5.
Table 3.1: Grid quality of the 3-D Model 1.

<p>| | |</p>
<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
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<tr>
<td>Maximum cell skewness</td>
<td>0.799897</td>
</tr>
<tr>
<td>Maximum aspect ratio</td>
<td>1.74976</td>
</tr>
</tbody>
</table>

Table 3.2: Grid size of 3-D Model 1.

<p>| | |</p>
<table>
<thead>
<tr>
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</thead>
<tbody>
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<td>Cells</td>
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<td>Cell zones</td>
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<td>Face zones</td>
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</tr>
</tbody>
</table>

Figures 3-5 and 3-6 show details of the grid.
Figure 3-5: 3-D Model 1 Grid Details

Figure 3-6: 3-D Model 1 Grid Cross Section
3.1.3. Numerical setup and physics

The Table 3.3 shows the most important numerical schemes and physical models used in 3-D model 1. The detailed description is in Chapter 2.

Table 3.3: Numerical and geometrical setup parameters of model 1.

<table>
<thead>
<tr>
<th>Solver type:</th>
<th>Pressure based 3D double precision</th>
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<tr>
<td>Simulation type:</td>
<td>Steady state calculations</td>
</tr>
<tr>
<td>Velocity formulation:</td>
<td>Absolute</td>
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<tr>
<td>Gradient option:</td>
<td>Green-Gauss Cell Based</td>
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<tr>
<td>Turbulence model:</td>
<td>Realizable k-ε turbulence model</td>
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<tr>
<td></td>
<td>with standard wall functions</td>
</tr>
<tr>
<td>Multiphase model:</td>
<td>VOF model, 2-phases: air and liquid</td>
</tr>
<tr>
<td></td>
<td>(water)</td>
</tr>
<tr>
<td>Momentum, turbulent kinetic energy, and turbulent dissipation rate discretization method</td>
<td>Third order MUSCL</td>
</tr>
<tr>
<td>Volume fraction discretization method:</td>
<td>Modified HRIC</td>
</tr>
<tr>
<td>Pressure-velocity coupling:</td>
<td>Phase coupled SIMPLE</td>
</tr>
<tr>
<td>Residual absolute criteria:</td>
<td>$10^{-5}$ for continuity and $10^{-3}$ for velocities, k, ε, and water volume fraction</td>
</tr>
<tr>
<td>Grid type and size:</td>
<td>277148 tetragonal-hybrid cells</td>
</tr>
</tbody>
</table>
3.1.4 Numerical validation

3.1.4.1. Numerical residuals

The criterion for convergence was that residuals have to fall below $10^{-3}$ for all properties. When the simulation converged, following residuals were recorded:

- Continuity: $5.67 \times 10^{-6}$
- x-velocity: $8.22 \times 10^{-4}$
- y-velocity: $5.91 \times 10^{-4}$
- z-velocity: $6.99 \times 10^{-4}$
- k: $9.18 \times 10^{-4}$
- $\varepsilon$: $9.55 \times 10^{-4}$

The results show that all residuals fell below values specified by convergence criterion.
In order to check grid dependence, after the simulation converged, the results of important fluid quantities are recorded to be compared with results when the grid is refined. The selected quantities are representative of turbulence, numerical convergence and multiphase fluid flow field:

- Mass-weighted average turbulent kinetic energy (k)
- Mass-weighted average turbulent intensity
- Mass-weighted average turbulent dissipation rate (ε)
- Mass-weighted average velocity magnitude
- Mass-weighted average mass imbalance
- Mass-weighted average volume fraction of air
- Mass flowrate through a selected reference plane.
The results are shown in Table 3.4.

Table 3.4: Selected Flow Properties Results.

<table>
<thead>
<tr>
<th>Mass-weighted average turbulent kinetic energy (k) m²/s²)</th>
<th>17.59628</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass-weighted average turbulent intensity (%)</td>
<td>296.9694</td>
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<tr>
<td>Mass-weighted average turbulent dissipation rate (ε) m²/s³)</td>
<td>9241.458</td>
</tr>
<tr>
<td>Mass-weighted average velocity magnitude (m/s)</td>
<td>17.41312</td>
</tr>
<tr>
<td>Mass-weighted average mass imbalance (kg/s)</td>
<td>-1.955828×10⁻¹⁰</td>
</tr>
<tr>
<td>Mass-weighted average volume fraction of air</td>
<td>0.9795452</td>
</tr>
<tr>
<td>Mass flow rate through the reference plane (kg/s)</td>
<td>2.010865</td>
</tr>
</tbody>
</table>
3.1.4.2 Grid Dependence Study

To numerically validate this model, a grid dependence study was performed. Two other grids, each finer than the grid described in section 3.1.1, were built and named “Dense Grid 1” and “Dense Grid 2”. In short, Dense Grid 1 has about 2.7 times more cells than the original grid, while Dense Grid 2 has about 3.76 times more cells than the original grid. Results for selected flow properties were compared after simulations converged, which took about 390 000 iterations. In the following sections grid quality, mesh size and comparison of flow properties are presented.

3.1.4.2.1 Results for Dense Grid 1

Figure 3-7: 3-D model 1 Cross Section of Dense Grid 1
Figure 3-7 shows cross section of Dense Grid 1.

Table 3.5: Dense Grid 1 Grid Quality

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</table>

Table 3.6: Dense Grid 1 Grid Size

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<td><strong>face zones</strong></td>
<td>9</td>
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Table 3.7: Selected Flow Properties Results for Dense Grid 1.

<table>
<thead>
<tr>
<th>Mass-weighted average turbulent kinetic energy (k) m$^2$/s$^3$</th>
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<tbody>
<tr>
<td>Mass-weighted average turbulent intensity (%)</td>
<td>294.79007</td>
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<tr>
<td>Mass-weighted average turbulent dissipation rate (ε) m$^2$/s$^3$</td>
<td>14159.914</td>
</tr>
<tr>
<td>Mass-Weighted Average Velocity Magnitude (m/s)</td>
<td>18.778023</td>
</tr>
<tr>
<td>Mass-Weighted Average Mass Imbalance (kg/s)</td>
<td>-1.4966362·10$^{-10}$</td>
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<tr>
<td>Air Mass-Weighted Average Volume fraction</td>
<td>0.96288543</td>
</tr>
<tr>
<td>Mass flow rate through reference plane (kg/s)</td>
<td>1.99462</td>
</tr>
</tbody>
</table>
3.1.4.2.2 Results for Dense Grid 2

Figure 3-8 show cross section of Dense Grid 2.

Figure 3-8: 3-D model 1 cross section of dense grid 2

Table 3.8: Dense Grid 2 Grid Quality.

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Table 3.9: Dense Grid 2 Grid Size.

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<td><strong>cell zones</strong></td>
<td>1</td>
</tr>
<tr>
<td><strong>face zones</strong></td>
<td>9</td>
</tr>
</tbody>
</table>
Table 3.10: Selected Flow Properties Results for Dense Grid 2.

<table>
<thead>
<tr>
<th>Mass-weighted average turbulent kinetic energy (k) m²/s²</th>
<th>17.561227</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass-weighted average turbulent intensity (%)</td>
<td>291.79341</td>
</tr>
<tr>
<td>Mass-weighted average turbulent dissipation rate (ε) m²/s³</td>
<td>14040.673</td>
</tr>
<tr>
<td>Mass-weighted average velocity magnitude (m/s)</td>
<td>18.882834</td>
</tr>
<tr>
<td>Mass-weighted average mass imbalance (kg/s)</td>
<td>1.203517×10⁻¹⁰</td>
</tr>
<tr>
<td>Air mass-weighted average volume fraction</td>
<td>0.96243969</td>
</tr>
<tr>
<td>Mass flowrate through reference plane (kg/s)</td>
<td>2.023861</td>
</tr>
</tbody>
</table>
The following differences between results of Dense Grid 1 and Dense Grid 2 were calculated as following:

- Mass-Weighted Average Turbulent Kinetic Energy: 1.7 %
- Mass-Weighted Average Turbulent Intensity: 1 %
- Mass-Weighted Average Turbulent Dissipation Rate: 0.85 %
- Mass-Weighted Average Velocity Magnitude: 0.55 %
- Air Mass-Weighted Average Volume Fraction: 0.046 %
- Mass flow rate through reference plane: 1.4 %

The difference is less than 1.5 % for all properties, which is acceptable.
3.1.5 Results of the 3-D Model 1

Figure 3-9: Pathlines of Liquid Droplets Colored by Droplet Number.

Pathlines in Figure 3-9 show that the fluid enters through the orifice at the lower right side of the picture, gets into the contact with the wheel and then a part of it goes between the wheel and the grinded part and rest of it is deflected to the sides or sticks to the wheel until rejected by the centrifugal forces (note the spiral pathlines of the fluid on the sides of the wheel). Tracking of fluid particles is especially interesting in understanding the flow patterns and determining the amount of used vs. wasted grinding fluid.

Figures 3-10 to 3-13 shows the isometric view of vectors of velocity of the grinding liquid. The highest velocities are present in the region between the wheel and the grinded part. Two diverging fluid streams, deflected to the sides can be clearly seen (rejected, or wasted part of the flow). A part of the liquid is entrained by the wheel and later rejected.
by high centrifugal forces. Sticking of the liquid to the grinding wheel is evident in the figures. The fluid entrained by the wheel is brought into the grinding region which helps in increasing the amount of the fluid that flows through the grinding zone (useful flowrate).

Figure 3-10: Isometric View of Velocity Vectors Colored by Velocity Magnitude [m/s].

In Fig. 3-10 regions of high speed flow can be clearly seen as being of reddish color. The highest velocity is present in the grinding region, and green-colored rejected flow can be seen to exit the domain through the side boundaries.

In Figures 3-11 to 3-13 the most important features of the flow field are indicated. These features are: inlet jet (by which metalworking fluid enters the domain), flow inside the grinding region (useful flow), rejected flow (mostly wasted), exit jet (flow which exits the grinding region), flow entrained by the wheel and flow deflected by the shield.
Figure 3-11: Bottom View of Velocity Vectors Colored by Velocity Magnitude [m/s].

Figure 3-12: Side View of Velocity Vectors Colored by Velocity Magnitude [m/s].
Figure 3-13: Front of Velocity Vectors Colored by Velocity Magnitude [m/s].

Figure 3-14: a) Velocity Contours of Air [m/s], b) Velocity Vectors of Air [m/s].

Figure 3-14 refers to the cross section of the computational domain along the symmetry plane of the domain (oriented in x-y directions). Formation of the boundary layer of air around the wheel (a) and interaction of that boundary layer with the inlet jet in the zoomed region close to the liquid inlet (b) can be seen in the figure. Air is set in
motion by the high-speed wheel. The boundary layer hits the edge of the top left part of the domain (solid wall – shield) and gets thinner. This obstruction is similar to the effect of an air scraper. After that, the boundary layer increases in size again. In figure 3-14 b, velocity vectors of air clearly indicate that high speed air hits the inlet jet from the top thus changing its direction and ability to penetrate the gap region between the wheel and the grinded part.

Figure 3-15 shows contours of the liquid velocity on solid surfaces. It can be seen that fluid on the shield and workpiece is colored by blue, which indicates that no-slip condition requirement is satisfied (those two solid surfaces do not move, and because of the no-slip condition, fluid sticks to the wall and is motionless). The flow on the wheel conforms to the no-slip condition, too, but the wheel spins with a constant angular velocity. The angular velocity of the wheel, multiplied by the distance between the center of wheel side surface, results in tangential velocity of the fluid particles that stick to the wheel. Therefore, the coloration of the fluid velocity contours correspond to the increasing tangential velocity as the position of the fluid particle is increased from the center to the rim of the wheel.
Figure 3-15: Velocity Contours of the Liquid Colored by the Velocity Magnitude [m/s].

Figure 3-16: Turbulence Intensity Contours [%]
3.1.6 Boundary Conditions for 3-D Model 2

After obtaining the global fluid flow in the 3-D Model 1, the results are used to generate detailed boundary conditions for the 3-D Model 2 in addition to a better understanding of the flow around the wheel. Three planes (named Plane 1, Plane 2 and Plane 3), which correspond to edges of geometry of 3D Model 2, were created in order to capture essential fluid flow quantities necessary for specifying boundary conditions. Those quantities are:

- Static pressure
- Turbulent kinetic energy
- Turbulent dissipation rate

It should be noted that by changing the flow in the grinding zone (3-D Model 1 vs. 3-D Model 2), the flow conditions at the boundaries of the 3-D Model 2 change as well. Therefore, the boundary conditions obtained from the 3-D Model 1 are an approximation of the real boundary conditions. But this approach is much better that just guessing the flow values at the boundaries. The care has been taken that physics and numerics of the 3-D Model 1 are not very different from the 3-D Model 2 so that the generated boundary conditions closely resemble the real flow values at the boundaries of 3-D Model 2. The boundaries of 3-D Model 2 are positioned well away from the grinding zone, in order to minimize their influence on the flow in the grinding zone.

Figures 3-17, 3-18 and 3-19 show planes used to capture boundary conditions for 3-D Model 2.
Figure 3-17: Plane 1 – Used for the Boundary Conditions at the Front of 3-D Model 2.

Figure 3-18: Plane 2 – Used for the Boundary Conditions at the Top of 3-D Model 2.
Figure 3-19: Plane 3 – Used for the Boundary Conditions at the Sides of 3-D Model 2.
3.2 3-D Model 2

3.2.1 Description of the Geometry

The general geometry contains a part of grinding wheel, workpiece, coolant inlet, outlet boundaries and porous grinding zone (simulated as a porous region with heat generation and particle injection). Two different sub-geometries were created, in order to comply with setups of experiments in selected journal papers.

3.2.1.1 Geometry 1

Geometry 1 corresponds to an example of deep grinding. Wheel diameter is 340 mm, wheel width is 50 mm, grinding zone size is: 0.03 m in x-direction, 0.03 m in y direction, and 0.001 m in z-direction (grinding depth). Porosity of the grinding zone is chosen as 0.5 which corresponds to the mid-range of commercially available wheels.

The size of the whole domain is:

- Minimum x coordinate = -0.05 m
- Maximum x coordinate = 0.08 m
- Minimum y coordinate = - 0.09999999 m
- Maximum y coordinate = 0.09999999 m
- Minimum z coordinate = -0.171 m
- Maximum z coordinate = -0.155 m
Figures 3-20 to 3-22 show in detail the most important parts of Geometry 1, such as: grinding wheel, porous grinding region, coolant inlet and workpiece.

Figure 3-20: Solid Surfaces and Porous Grinding Region of 3-D Model 2 Geometry 1.

Figure 3-21: Outline and Grinding Region of 3-D Model 2 Geometry 1.
Figure 3-22: Zoomed View of Grinding Region and Grinding Wheel of 3-D Model 2

Geometry 1.
3.2.1.2 Geometry 2

Geometry 2 corresponds to an example of shallow-cut grinding. In order to decrease the time required for the simulations, this geometry represents only a half of the full geometry, and the symmetry boundary condition is applied at the side which corresponds to the symmetry plane of the full geometry. Wheel diameter is 202 mm, wheel width is 19 mm, grinding zone size is: 0.0025 m in x-direction, 0.0095 m in y direction, and 0.0001 in z-direction. Porosity of the grinding zone is chosen as, once again, 0.5 which corresponds to the mid-range of commercially available wheels.

The size of the whole domain is:

- Minimum x coordinate = -0.05 m
- Maximum x coordinate = 0.08 m
- Minimum y coordinate = 0.2 m
- Maximum y coordinate = 0.3 m
- Minimum z coordinate = -0.171 m
- Maximum z coordinate = -0.155 m

Figures 3-23 and 3-24 show in detail the most important parts of Geometry 2, such as: grinding wheel, porous grinding region, coolant inlet and workpiece.

Comparing the Figures 3-21 and 3-23 it can be seen that the size of the grinding region in Geometry 2 is much smaller than in Geometry 1.
Figure 3-23: Outline and grinding region of 3-D model 2 geometry 2

Figure 3-24: Outline Zoomed view of grinding region and grinding wheel of 3-D model 2 geometry 1
3.2.2 Grid Properties

3.2.2.1 Grid Properties for Geometry 1

Table 3.11: Grid Quality for Geometry 1.

<p>| | |</p>
<table>
<thead>
<tr>
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<th></th>
</tr>
</thead>
<tbody>
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<tr>
<td><strong>Maximum cell skewness</strong></td>
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<tr>
<td><strong>Maximum aspect ratio</strong></td>
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</table>

Table 3.12: Grid Size for Geometry 1.

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<th></th>
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</thead>
<tbody>
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</tr>
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<tr>
<td><strong>cell zones</strong></td>
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</tr>
<tr>
<td><strong>face zones</strong></td>
<td>28</td>
</tr>
</tbody>
</table>

Figures 3-25 to 3-28 show grid details for 3-D Model 2 Geometry 1. In Fig. 3-27 it can be seen that the grid size is much finer in the contact region in order to correctly capture the flow features.
Figure 3-25: Grid for 3-D Model 2 Geometry 1

Figure 3-26: Zoomed View of Grid of Grinding Region for 3-D model 2 geometry 1.
Figure 3-27: Cross Section of Grid of 3-D Model 2 Geometry 1.

Figure 3-28: Boundary Layer Grid in Grinding Region
Figure 3-28 shows the boundary layer grid in the grinding region which is necessary because the velocity gradients are very large close to the solid boundaries. The rest of the workpiece and grinding wheel were covered by the boundary layer grid as well.

3.2.2.2 Grid Properties for Geometry 2

Table 3.13: Grid Quality for geometry 2.

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</table>

Table 3.14: Grid Size for Geometry 2.

<p>| | |</p>
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<thead>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
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<tr>
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<td>cell zones</td>
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<td>face zones</td>
<td>25</td>
</tr>
</tbody>
</table>

Figures 3-29 and 3-30 show grid details for 3-D Model 2 Geometry 2. Similarly to the Geometry 1, fine grids in the grinding zone and boundary layer grind were applied.
Figure 3-29: Grid for 3-D model 2 geometry 2

Figure 3-30: Cross section of mesh of 3-D model 2 geometry 2
3.2.3 Numerical setup and physics

The model applies high-resolution schemes in order to correctly capture essential features of fluid flow and heat transfer. Particular importance is given to application of High Resolution Interface Capturing (HRIC) schemes [21] which give the most accurate prediction of position of liquid-gas interface. In Table 3-16 list of discretization schemes is presented.

The objective for 3-D Model 2 is to study in detail the fluid flow and heat transfer in the abrasive contact region and its vicinity. It is well known that fluid which entered in the wheel pores before the grinding zone will be carried through the abrasive contact [1]. The conjecture that the fluid is able to (at least partially) penetrate inside the wheel porosity represents a key component of the fluid flow, with a profound impact on the grinding process itself. Compared to the previous phase and building upon it, in this phase of the study the wheel has a known porosity. The fluid is able to penetrate the wheel in the regions of high-pressure and be ejected from the wheel in the regions of low external pressure because of the centrifugal acceleration. Unlike the previous case, the effect of surface tension was included.

The model consists of 3-D geometry with grinding wheel, workpiece and detailed contact zone. The key to modeling the abrasive contact region between the grinding wheel and the workpiece was the introduction of a porous zone, corresponding to the abrasive contact (the thickness of the fluid film in the contact region). The idea was to describe the flow in the contact zone as a flow through a porous medium. The reasoning behind this is that in the real contact zone, at a given time, a limited number of grains
make contact with the workpiece. This generates a complex labyrinth of passages through which the coolant must flow. The fluid changes direction, separates, and in the end loses energy encountering all those resistances. Equivalent phenomena happen to a fluid which flows through a porous zone, so an analogy can be established. On the other hand, the fluid receives kinetic energy from the high-speed motion of the grinding wheel. This aspect is represented by the fact that the porous region will be considered as moving with the tangential velocity of the wheel. When the porous media model is used, a zone must be defined in which the porous media model is applied and the pressure loss in the flow is determined via user inputs as it is described.

Heat transfer through the medium was also represented, subject to the assumption of thermal equilibrium between the medium and the fluid flow - steady distributions. The modeling of porous media was done by the addition of a momentum sink term to the Navier-Stokes equations. The sink term contains two parts: Darcy’s viscous loss term (the first term on the right-hand side of the Eq. (3.1)) and an inertial loss term (the second term on the right-hand side of the Eq. (3.1)) [10]:

\[
S_i = \left( \sum_{j=1}^{3} D_{ij} \cdot \mu \cdot v_j + \sum_{j=1}^{3} C_{ij} \cdot \frac{1}{2} |v| \cdot v_j \right),
\]

where:

- \( S_i \) is the source term for the i-th (x, y or z) momentum equation,
- \( |v| \) is the magnitude of velocity
- D and C are prescribed matrices representing the properties of the porous medium, which must be measured or theoretically predicted.
This momentum sink contributes to the pressure gradient in the porous cell, creating a pressure drop that is proportional to the fluid velocity (Darcy’s viscous loss term), or velocity squared (the inertial loss term) in the cell [10]. The FLUENT software also allows the sink term to be modeled more generally as a power law of the velocity magnitude [10]:

$$S_i = -C_0 \cdot |v|^C = -C_0 \cdot |v|^{(C_i-1)} \cdot v_i,$$

where $C_0$ and $C_i$ are user-defined empirical coefficients. At high flow velocities, coefficients $C_{ij}$ provide corrections for inertial losses in the porous medium. Any such coefficient can be viewed as a loss coefficient per unit length along the flow direction, thereby allowing the pressure drop to be specified as a function of the dynamic head [10]. The software solves the standard energy transport equation in porous media regions with modifications to the conduction flux and the transient terms. In the porous medium, the conduction flux uses an effective conductivity and the transient term includes the thermal inertia of the solid region on the medium [10]:

$$\frac{\partial}{\partial t} \left( \gamma \cdot \rho_f \cdot E_f + (1-\gamma) \cdot \rho_s \cdot E_s \right) + \nabla \cdot \left( \nabla \left( \rho_f \cdot E_f + p \right) \right) =$$

$$= \nabla \cdot \left[ k_{\text{eff}} \cdot \nabla T - \left( \sum_i h_i \cdot J_i \right) + \left( \frac{\mathbf{f}}{\rho} \cdot \mathbf{v} \right) \right] + S^h_f$$

The fluid temperature dependent thermal conductivity $k_f$ and the solid thermal conductivity $k_s$ can be computed via user-defined functions. The anisotropic effective thermal conductivity can also be specified via user-defined functions. In this case, the isotropic contributions from the fluid, $\gamma \cdot k_f$, are added to the diagonal elements of the solid anisotropic thermal conductivity matrix [10].
In this work, packed beds porosity model was used in the porous grinding region due to the shape of grain-workpiece contacts in grinding region. The model uses permeability and inertial loss coefficients [10]. The derivation of the model involves Ergun and Darcy equations. The Ergun equation [52] is a semi-empirical correlation that can be applied for flows characterized by a broad range of Reynolds numbers and can be written as follows [52]:

\[
\frac{|\Delta p|}{L} = \frac{150 \cdot \mu}{D_p^2} \cdot \frac{(1 - \varepsilon)^2}{\varepsilon^3} \cdot v_\infty + \frac{1.75 \cdot \rho}{D_p} \cdot \frac{(1 - \varepsilon)}{\varepsilon^3} \cdot v_\infty^2,
\]

(3.4)

where:

- \( \mu \) is the fluid viscosity,
- \( D_p \) is the mean particle diameter (grain size, in this work)
- \( L \) is the bed depth (length of the grinding region, in this work)
- \( \varepsilon \) is the void fraction - the volume of voids divided by the total volume of the packed bed region (wheel porosity in this work).

Darcy's Law can be expressed as [10]:

\[
\nabla p = -\frac{\mu}{\alpha} \cdot \vec{v},
\]

(3.5)

Where \( \alpha \) is permeability.

A simplification of the porous media equation can be written as [10]:

\[
\nabla p = -\sum_{j=1}^{3} C_{2ij} \cdot \left( \frac{1}{2} \cdot \rho \cdot v_j \cdot |v| \right).
\]

(3.6)
By combining Eqs. (3.4) to (3.6), the equations for calculation permeability and inertial loss coefficients can be expressed as [10]:

$$\alpha = \frac{D_p^2}{150} \frac{\varepsilon^3}{(1-\varepsilon)^2}, \quad (3.7)$$

and:

$$C_2 = \frac{3.5}{D_p} \frac{(1-\varepsilon)}{\varepsilon^3}. \quad (3.8)$$

3.2.3.1 Choosing the Turbulence Model

The choice of turbulence model depends on the geometry and complexity of the flow field in the computational domain. The class of problems encountered in this work contains a wide range of length and time scales, stationary and moving wall boundaries, porous regions and complex geometries, especially in the contact region. Due to the mentioned complexity, and the results of the parametric study performed in this work, the Reynolds stress model was chosen. RSM abandons the isotropic eddy viscosity hypothesis, which is used in k-\(\varepsilon\) and k-\(\omega\) models for example, and closes the Reynolds-averaged Navier-Stokes equations by solving transport equations for the Reynolds stresses, together with an equation for the dissipation rate. This means that five additional transport equations are required in 2D flows and seven additional transport equations must be solved in 3D. Since the RSM accounts for the effects of streamline curvature,
swirl, rotation, and rapid changes in strain rate in a more rigorous manner than one-equation and two-equation models, it has greater potential to give accurate predictions for complex flows. So, the use of the RSM is a must when the flow features of interest are the result of anisotropy in the Reynolds stresses, such as in this case (in grinding). In order to compare performance of RSM model, a parametric study was performed in which results of two more turbulence models were investigated in section 3.2.6.3.

3.2.3.2 Heat Generation and Transfer

The heat generation, distribution of heat sources and temperature distribution was also examined. Grinding power is converted into heat, chip acceleration and material deformation. A negligible part of this power accelerates the chip and a very small proportion is locked into the deformed material. The most of the input energy in grinding goes into heat generation. Heat generation was modeled as a heat generation surface at the contact between the grinded part and the grinding wheel, thus mimicking the real-world heat generation. In reality there are small contacts between the grain features on the wheel and the grinded part. The main sources of heat in grinding were shown to be those grain-workpiece rubbing surfaces [14]. The size of these contacts can be determined from the size of the grains and the geometry of the grinding. Each of contacts represents a heat source. When added up, they represent the total heat source whose strength is the same as heat generation surface in the described model.

The geometrical parameters of the wheel were determined by using average grain size and distribution, using the ANSI specifications. The wheel was modeled as two
cylindrical shapes one inside another: non-permeable core and the porous part of the wheel in contact with the grinding zone. The ANSI standard gives a measure of wheel mesh size. Each grain size for conventional abrasives is specified with reference to the mesh number of sieves used in sorting the grains. The mesh number indicates the number of wires per inch in the sieve. A larger mesh number indicates a smaller grit dimension. Malkin [15] gives approximate relationships to relate average grain size $d_g$ to mesh number $M$:

$$d_g = \frac{15.2}{M} [\text{mm}] \quad (3.9)$$

The average grain spacing may be assumed as:

$$C_{av} = \frac{1}{2.25 \cdot d_g^2}. \quad (3.10)$$

As mentioned, contact between each grain and workpiece surface represents an elementary heat source. If all of them are added up, the total heat source strength is calculated. In our model we input that energy into the bottom of the porous contact zone.

The strength of an elementary heat source, $Q_{iz}$, can be expressed as [16]:

$$Q_{iz} = F_w \cdot v_t \cdot t_z, \quad (3.11)$$
where:

- \( F_{ze} = \frac{F_{vm}}{N_a \cdot A_k} \) is the main grinding force (\( F_{vm} \) is total main grinding force, \( N_a \) is number of active grains per unit of surface of grinding wheel, \( A_k \) is the contact surface area between grinding wheel and grinded part),
- \( v_t \) is grinding wheel circumferential velocity,
- \( t_z = \frac{\sqrt{a \cdot D_t}}{v_t} \) is period of time during which grain cuts the workpiece (\( a \) is grinding depth, \( D_t \) is diameter of grinding wheel).

The total strength of the heat source is [16]:

\[
Q = Q_{tz} \cdot N_a \cdot A_k. \tag{3.12}
\]

Combining previous equations yields [16]:

\[
Q = F_{vm} \cdot v_t \cdot t_z. \tag{3.13}
\]

In grinding, parameters of the process are usually expressed per contact unit width, \( b_k \), so the previous equation can be transformed into [16]:

\[
Q' = F'_{vm} \cdot v_t \cdot t_z, \tag{3.14}
\]

where:

- \( Q' = \frac{Q}{b_k} \) is specific strength of the heat source
- \( F'_{vm} = \frac{F_{vm}}{b_k} \) is specific main grinding force.
The specific main grinding force can be expressed using the equation [16]:

\[ F_{vm} = h_m \cdot k_{vm}, \]  
(3.15)

where:

- \( h_m = \frac{v_p}{v_i} \cdot a \) is mean chip thickness
- \( v_p \) is workpiece velocity,
- \( k_{vm} \) is specific main grinding resistance.

Therefore [16]:

\[ F_{vm} = \frac{v_p}{v_i} \cdot a \cdot k_{vm}. \]  
(3.16)

The final equation for the total heat source strength is obtained by combining equations (3.14) to (3.16) [16]:

\[ Q = \frac{v_p}{v_i} \cdot a^{\frac{3}{2}} \cdot D_i^{\frac{1}{2}} \cdot k_{vm}. \]  
(3.17)

The specific main grinding resistance was calculated using the equation [16]:

\[ k_{vm} = \frac{C_k}{\sqrt{A}}. \]  
(3.18)

Parameters \( C_k \) and \( \varepsilon_k \) for common materials are presented in table 3.15.
Table 3.15. Parameters for the Calculation of the Specific Main Grinding resistance for Common Materials [17].

<table>
<thead>
<tr>
<th>Material</th>
<th>$C_k$</th>
<th>$\varepsilon_k$</th>
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</thead>
<tbody>
<tr>
<td>Cast iron</td>
<td>$1.448\cdot10^8$</td>
<td>7.4</td>
</tr>
<tr>
<td>Carbon steel</td>
<td>$1.936\cdot10^8$</td>
<td>6.1</td>
</tr>
<tr>
<td>Chrome-nickel steel</td>
<td>$6.263\cdot10^8$</td>
<td>10.4</td>
</tr>
<tr>
<td>Cast steel</td>
<td>$2.196\cdot10^8$</td>
<td>6.7</td>
</tr>
<tr>
<td>Bronze</td>
<td>$0.248\cdot10^8$</td>
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</tr>
<tr>
<td>Brass</td>
<td>$0.9\cdot10^8$</td>
<td>6.8</td>
</tr>
<tr>
<td>Aluminum</td>
<td>$1.92\cdot10^8$</td>
<td>8</td>
</tr>
</tbody>
</table>

3.2.3.3 Motion considerations

The relative motion between grinding wheel and grinded part motion was approximated by using multiple rotating reference frame technique available in FLUENT. The domain was separated into 2 parts: rotational reference frame next to the grinding wheel and stationary reference frame next to the grinded part. This technique is a reliable tool for simulating time-averaged flow fields.
Table 3.16 contains additional numerical settings of this model.

Table 3.16. Numerical setup parameters for the model 2.

<table>
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<tr>
<th>Parameter</th>
<th>Setting</th>
</tr>
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<tr>
<td><strong>Simulation type:</strong></td>
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</tr>
<tr>
<td><strong>Velocity formulation:</strong></td>
<td>Absolute</td>
</tr>
<tr>
<td><strong>Gradient option:</strong></td>
<td>Green-Gauss Cell Based [18]</td>
</tr>
<tr>
<td><strong>Turbulence model:</strong></td>
<td>Reynolds Stress Model [19]</td>
</tr>
<tr>
<td><strong>Multiphase model:</strong></td>
<td>(VOF) 2-phase model (liquid and gas), which includes surface tension and wall adhesion</td>
</tr>
<tr>
<td><strong>Momentum, turbulent kinetic energy, turbulent dissipation rate, Reynolds stresses and energy equation discretization method:</strong></td>
<td>Third order MUSCL [20]</td>
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<tr>
<td><strong>Pressure discretization method:</strong></td>
<td>Body-force weighted</td>
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<tr>
<td><strong>VOF discretization method:</strong></td>
<td>High Resolution Interface Capturing [21]</td>
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<td><strong>Porous zone motion:</strong></td>
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<td><strong>Pressure-velocity coupling:</strong></td>
<td>Phase coupled SIMPLE [22]</td>
</tr>
<tr>
<td><strong>Residual absolute criteria:</strong></td>
<td>$10^{-6}$ for energy and $10^{-3}$ for velocities, $k$, $\epsilon$, water volume fraction and continuity</td>
</tr>
<tr>
<td><strong>Grid type and size:</strong></td>
<td>2063714 tetragonal cells</td>
</tr>
</tbody>
</table>
3.2.4 Numerical validation

Mass imbalance:

- whole model mass flow rate imbalance equals 0.00007% of total flow rate (below acceptable 0.2% - FLUENT recommendations)

Numerical residuals were recorded when the simulation converged:

- continuity: $9 \cdot 10^{-4}$ (the convergence criterion was set to $10^{-3}$)
- energy: $1.1 \cdot 10^{-7}$ (the convergence criterion was set to $10^{-6}$)
- volume fraction of water: $5 \cdot 10^{-4}$ (the convergence criterion was set to $10^{-3}$)

In performed grid dependence study, a finer mesh with 2836284 cells was created. The difference in useful flowrate compared to the original grid was below 0.3 %.

3.2.5 Experimental validation

3-D Model 2 was verified regarding useful flow rates, maximum temperature change of grinding fluid in the abrasive region and static pressures on the centerline of the grinded part by comparing its results for several different wheel speeds and inlet flow rates to experimental results from selected paper.
3.2.5.1 Useful flow rates comparison

Comparison of useful flow rates was done for different inlet velocities and wheel velocities. 3-D Model 2 Geometry 1 was used. Important simulation parameters were:

- Inlet velocities [m/s]: 7.51, 17.54, 27.56, 38.08, 55.11
- Wheel velocities (\(W_v\)) [m/s]: 20.8, 41.6, 62.4
- Grinding depth = 1 mm
- Experimental data source: [6]

The comparison is shown in figure 3-31.

![Figure 3-31. Comparison of Numerical and Experimental Results for Useful Flowrates.](image)
The comparison shows that the numerical simulation results comply well with the experimental data and follow the trend of increasing the useful flowrate with increasing fluid inlet velocity.

3.2.5.2 Comparison of maximum change in fluid temperature

For this study, 3-D model 2 Geometry 1 was used. Experimental data can be found in [9]. The most important simulation parameters were:

- Wheel velocity = 20.4 m/s
- Grinding fluid inlet velocity = 15.5 m/s
- Heat input in the grinding zone [W/mm²]: 0, 2, 4, 6, 8
- Grinding depth = 1 mm

![Graph showing maximum change in temperature of grinding fluid during the grinding process](image)

Figure 3-32. Maximum Change in Temperature of Grinding Fluid During the Grinding.
The comparison is graphically shown in figure 3-32. The results of the simulation follow the nonlinear trend that is present in the experimental data. The experiments were not conducted for the case without energy input, because there would be no change in fluid temperature.

In practical application, the energy input to the model can be predicted by equation 3-17. Alternatively, it can be measured at the grinding machine.

3.2.5.3 Comparison of static pressures on the grinded part

For this study 3-D Model 2 Geometry 2 was used. The most important simulation parameters were:

- Wheel velocity = 20 m/s
- Grinding fluid inlet volume flowrate = 10 liters/min
- Grinding depth = 0.05 mm
- Wheel radius = 101 mm, wheel width = 19 mm
- Experimental data source: [23]

The comparison is graphically shown in Figure 3-33. Values obtained by simulations are quite close to the experiments and the curve trend is the same.
3.2.6 Model results and parametric studies

The numerical and experimental validations of the model showed that the satisfactory convergence and accuracy was obtained. All numerical residuals dropped below recommended levels and there were no stability problems. The average errors were: 1) for fluid flow rate comparison: 11.07 %, 2) for maximum change in fluid temperature: 6.64 %, 3) for static pressures: 25.35 %. The maximum static pressure was predicted with error of 2.44 %. The shapes of the curves for all three compared physical quantities, acquired from the simulations, closely follow corresponding experimental curves, showing that presented model captures nonlinear behaviors very well.
To illustrate the capability of the model, and to better understand how it works, a typical set of grinding parameters was used as an example of the model’s applicability. The spatial parameters used were from 3-D Model 2 Geometry 1: wheel diameter = 370mm, wheel width = 50mm, grinding depth = 1mm, nozzle diameter = 6mm, and nozzle flow rate is from 3 to 22 kg/sm. Water physical properties were used for the grinding fluid.

Figure 3-34 shows an isometric view of the velocity vector field. The fluid enters the domain from an inlet close to the upper right corner of the figure. It hits the wheel, and part is deflected and sprayed to the sides of the wheel (this part is shown in dark blue because of the low volume fraction of liquid, and it has no other contribution to the grinding process); the rest of the fluid is entrained by the rotating wheel and by the high speed air boundary layer which surrounds it and enters the grinding zone.

Figure 3-34. View of Fluid Velocity Vector Field Colored by Metalworking Fluid Volume Fraction.
The fluid entering the narrow porous region represents the most important part of the flow (useful flow, the yellow region in Fig. 3-34); this fluid is accelerated and then it is expelled with high speed at the exit. Some fluid adheres to the wheel, but it is gradually thrown out due to the centrifugal force. Sticking of the fluid to the wheel is captured by this model as a result of the surface tension effects implemented through the VOF model. Figure 3-34 indicates that the grinding region contains a significant volume fraction of liquid (about 70%), which helps in lubrication and cooling.

Figure 3-35 shows the complete vector field of velocities in the 3-D Model 2 Geometry 2 domain. Some of the highest velocities are also found in the grinding region, as shown in Figs. 3-36 and 3-37. These figures compare the flow patterns in the grinding zone obtained for two fluid supply mass flow rates (flow rates were obtained by changing the fluid supply velocity). All the other work parameters are the same in the two simulations. The comparison indicates that an increased supply velocity can generate higher fluid velocities in the grinding contact region.
Figure 3-35. Velocity Vectors of Metalworking Fluid Colored by the Velocity Magnitude [m/s].

Figure 3-36. Velocity Vectors of Grinding Fluid for Inlet Flowrate of 3 kg/sm [m/s].
Figure 3-37. Velocity Vectors of Grinding Fluid for Inlet Flowrate of 22 kg/sm [m/s]

Figure 3-38 shows the temperatures in the whole domain of 3-D Model 2 Geometry 1. Cool liquid flow (colored in blue) enters from the right, removes some of the heat generated in the zone and leaves the domain to the left side. Heating of the fluid is clear from the picture, due to temperature increase between the inlet and exit from the grinding zone. Interesting conclusion is that fluid temperature is higher close to the sides of the grinding region, probably because of the wheel side blockage which prevents cooling. Figure 3-39 shows temperature distribution in zoomed grinding region for a lower heat generation input compared to Figure 3-38, but other parameters were kept same. Thus, the maximum temperatures are lower.
Figure 3-38. Velocity Vectors of the Grinding Fluid Colored by the Temperature [K].

Figure 3-39. Velocity Vectors of the Grinding Fluid in the Grinding Region, Colored by the Temperature [K].
Figure 3-40. Contours of Temperature on the Workpiece [K].

Figure 3-41. Contours of Temperature on the Bottom of Grinding Region [K].
Figures 3-40 and 3-41 show temperature distributions on the workpiece and on the grinding region. The effect of increased temperatures close to the sides of the grinding region is evident, again.

The contours of gage pressure on the grinded part are shown in figure 3-42. It can be seen that maximum pressures occur in the grinding region, while the rest of the workpiece is at atmospheric pressure.

Figure 3-42. Gage Pressure on the Grinded Part and Grinding Wheel [Pa].

Figure 3-43 shows gage pressure on the wheel. It can be seen that the fluid in the zone before the grinding region slows down, and dynamic pressure is converted to static pressure which increases (white dots in the figure). Then, the flow enters the grinding region (red dots in the figure), and the pressure does not build up, which is compatible with research results of Malkin et al. [5]. At the exit of the grinding region, flow is
subjected to the ambient fluid, and therefore it drops to the value of atmospheric pressure (zero gage pressure).

Figure 3-43. Gage pressure on the wheel before grinding region (white) and in grinding region (red) [Pa].

3.2.6.1 Influence of nozzle flowrate on maximum temperature on workpiece

A parametric analysis of the influence of the nozzle flow rate on the maximum temperature is shown in figure 3-44. Wheel velocity was set to 60 m/s and heat generation input was $8 \cdot 10^8 \frac{W}{m^3}$. It can be seen that lower supply flow rates generate higher temperatures; on the other hand, as the flow rate is increased, a saturation effect occurs, which limits the cooling effect. This find was observed for all configurations.
3.2.6.2 Influence of Multiphase Models on the Usefull Flowrate

In order to determine the best multiphase model for 3D simulations a comparison of VOF and Eulerian approaches has been made. The fluid flow in grinding is very complex and encompasses several different characteristics in different parts of simulation domain:

- Jet flow from nozzle orifice to the contact zone
- Stratified/free surface flow on the workpiece and around it
- Breakup of a part of a jet into small droplets.
- Flow in porous grinding region
- Highly swirling flow around the grinding wheel.
Multiple flow regimes are encountered in the same case. The usual approach is to select the most interesting aspect of the flow and apply the model that is best suited for that aspect of the flow. For example, when selecting the multiphase model, the delivery of the fluid to the grinding region and the flow inside it correspond to VOF most closely (stratified liquid-gas flow), but the liquid distribution in the domain may be influenced by droplet formation. Figures 3-45 to 3-47 show comparative results between the two multiphase model simulations and experimental measurements. The following grinding setup was used: Wheel diameter = 370mm, wheel width = 50mm, grinding depth = 1mm, nozzle diameter = 6mm, wheel speeds: 20.8 m/s, 41.6 m/s and 62.4 m/s, all for different jet speeds.

Figure 3-45. Useful Flowrate vs. Nozzle Jet Speed for 20.8 m/s Grinding Wheel Speed.
Figure 3-46. Useful Flowrate vs. Nozzle Jet Speed for 41.6 m/s Grinding Wheel Speed.

Figure 3-47. Useful Flowrate vs. Nozzle Jet Speed for 62.4 m/s Grinding Wheel Speed.
Performed numerical simulations yielded different results for Eulerian and VOF models, compared to experimental values. But numerical result trends were similar to experimental data for all models. To better understand the difference between the applied turbulence models, Figs. 3-48 to 3-50 show errors calculated based on the difference between numerical and experimental results.

Figure 3-48. Errors for Useful Flowrate vs. Nozzle Jet Speed for 20.8 m/s Grinding Wheel Speed.
Figure 3-49. Figure 3-48. Errors for Useful Flowrate vs. Nozzle Jet Speed for 41.6 m/s Grinding Wheel Speed.
On the average, errors were:

- For 20.8 m/s wheel speed: 12.6% for Eulerian, 10.1% for VOF
- For 41.6 m/s wheel speed: 17.5% for Eulerian, 13.81% for VOF
- For 20.8 m/s wheel speed: 19.8% for Eulerian, 9.3% for VOF

In both multiphase models, the error showed an oscillation pattern as function of the inlet jet speed. The amplitudes of the oscillations decreased as the jet speed increased. It is clear that VOF model outperforms Eulerian model, especially at high wheel velocities. Closer performance of VOF model to experimental results is probably due to incorporated surface tension and wall adhesion effects which help in obtaining a more.
accurate prediction of flow patterns, especially breakup of metalworking jet that hits the wheel and the grinding region. It also seems that mixing of two fluids is not strong enough in order to approach Eulerian model assumptions.

3.2.6.3 Influence of turbulence models on useful flowrate

Performances of three different turbulence models were investigated: realizable k-epsilon, SST k-omega and Reynolds stress model. The flow in grinding is influenced by the fast spinning wheel, which introduces large streamline curvature and rotation effects, and presence of anisotropy in the Reynolds stress (swirling flow). Figures 3-51 to 3-53 show results for simulations based on the used turbulence models compared to experimental results.

The following grinding setup was used: Wheel diameter = 370mm, wheel width = 50mm, grinding depth = 1mm, nozzle diameter = 6mm, wheel speeds: 20.8 m/s, 41.6 m/s and 62.4 m/s, all for different jet speeds.
Figure 3-51. Useful Flowrate vs. Nozzle Jet Speed for 20.8 m/s Grinding Wheel Speed.

Figure 3-52. Useful Flowrate vs. Nozzle Jet Speed for 41.6 m/s Grinding Wheel Speed.

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Performed numerical simulations yielded different results for different turbulence models, compared to experimental values. To compare the differences between the four sets of results, the Figs. 3-54 to 3-56 show relative errors.
Figure 3-54. Errors for useful flowrate vs. nozzle jet speed for grinding wheel speed of 20.8 m/s
Figure 3-55. Errors for useful flowrate vs. nozzle jet speed for grinding wheel speed of 41.6 m/s
Figure 3-56. Errors for useful flowrate vs. nozzle jet speed for grinding wheel speed of 62.4 m/s

On the average, errors were:

- For 20.8 m/s wheel speed: 15.6% for realizable $k$-$\varepsilon$, 16.5% for SST $k$-$\omega$, 10.1% for RSM
- For 20.8 m/s wheel speed: 21.0% for realizable $k$-$\varepsilon$, 24.4% for SST $k$-$\omega$, 13.8% for RSM
- For 20.8 m/s wheel speed: 12.4% for realizable $k$-$\varepsilon$, 24.1% for SST $k$-$\omega$, 9.3% for RSM

Results show that Reynolds stress model yielded the most accurate results over a wide range of wheel and jet velocities, while $k$-$\varepsilon$, and especially $k$-$\omega$ model tended to
overpredict the useful flow rate. More accurate performance of Reynolds stress model can be attributed to superior Reynolds stress transport model versus Boussinesq approach used in k-ε and k-ω models. A disadvantage of the realizable k-ε model is in producing non-physical turbulent viscosities in flows when the computational domain includes both rotating and stationary fluid zones, and that could be the reason it underperformed in the simulations.

3.2.6.4 Influence of Specific Heat on the Useful Flowrate and Temperatures

Specific heat is an intensive property of a substance and is defined as “the energy required to increase the temperature of a unit mass of a substance by one degree” [25]. It influences the ability of a metalworking fluid to cool, thus lowering temperatures in both tool and workpiece, reducing wear, quality of workpiece surface and allowing better control of the process.

The following grinding setup was used in this study: Wheel diameter = 370mm, wheel width = 50 mm, grinding depth = 1 mm, nozzle diameter = 6 mm, wheel speed: 20.8 m/s, jet speed: 7.51 m/s, heat generation in the contact zone: $10^{10}$ W/m$^3$. The fluid used in numerical simulation is water, with viscosity that linearly depends on temperature: 0.001002 Pa·s at 20°C, and 0.000282 Pa·s at 100°C. Viscosities out of that temperature range are linearly extrapolated. Figures 3-57 and 3-58 show influence of $C_p$ on average and maximum temperatures in the workpiece and useful flowrate.
Figure 3-57: Average and Maximum Temperatures on the Workpiece vs. Specific Heat of Metalworking Fluid.

Figure 3-58: Useful Flowrate vs. Specific Heat of Metalworking Fluid.
Indeed, Fig. 3-57 shows that a decrease of 3 times in \( C_p \) value from 6273 J/kg/K to 2091 J/kg/K resulted in 3.7 \% increase in maximum temperature and 10.7 \% increase in average temperature in the workpiece, so the influence of specific heat is not negligible. A decreased value of specific heat leads to a decreased capacity of the fluid to absorb thermal energy, thus leading to increased temperatures in the contact region. On the other hand, the flowrate increased for 0.93 \% only, as seen in Fig. 3.58.

3.2.6.4 Influence of Heat Conductivity on the Useful Flowrate and Temperatures

Heat conductivity (k) is ability of a substance to conduct heat. Thus, an increased k leads to a faster heat transfer to the fluid. Simulations were performed to show dependence of temperatures and useful flowrate on this physical property.

The following grinding setup was used in this study: Wheel diameter = 370 mm, wheel width = 50 mm, grinding depth = 1 mm, nozzle diameter = 6 mm, wheel speed: 20.8 m/s, jet speed: 7.51 m/s, heat generation in the contact zone: \( 10^{10} \) W/m\(^3\). The fluid used in numerical simulation is water, with viscosity that linearly depends on temperature: 0.001002 Pa·s at 20° C, and 0.000282 Pa·s at 100° C. Viscosities out of that temperature range are linearly extrapolated. Figures 3-59 and 3-60 show influence of k on average and maximum temperatures in the workpiece and useful flowrate.
Figure 3-59: Average and Maximum Temperatures on the Workpiece vs. Heat Conductivity of Metalworking Fluid.

Figure 3-60: Useful Flowrate vs. Heat Conductivity of Metalworking Fluid.
The results show that a 3 times decrease in heat conductivity value (from 0.9 to 0.3 W/m/K) resulted in very little change in temperatures in the workpiece: 0.63% increase in maximum temperature and 0.48% increase in average temperature. Similarly, the change in useful flowrate was very small: 0.41% increase. Thus, it can be concluded that \( k \) cannot be used as an effective property to control the temperature distribution in the grinding region.

3.2.6.5 Influence of Density on the Useful Flowrate and Temperatures

The total heat capacity of a fluid is linearly dependent on its density, so density was one of the parameters worth considering and analyzing, because of its presumed high impact on temperature field during grinding.

The following grinding setup was used: Wheel diameter = 370 mm, wheel width = 50 mm, grinding depth = 1 mm, nozzle diameter = 6 mm, wheel speed: 20.8 m/s, jet speed: 7.51 m/s, heat generation in the contact zone: \( 10^{10} \) W/m\(^3\). The fluid used in numerical simulation is water, with viscosity that linearly depends on temperature: 0.001002 Pa·s at 20° C, and 0.000282 Pa·s at 100° C. Viscosities out of that temperature range are linearly extrapolated. Figures 3-61 and 3-62 show influence of metalworking fluid density on average and maximum temperatures in the workpiece and useful flowrate.
Figure 3-61: Average and Maximum Temperatures on the Workpiece vs. Density of Metalworking Fluid.

Figure 3-62: Useful Flowrate vs. Density of Metalworking Fluid
The Fig. 3-61 shows that a 3 times decrease of density increased maximum temperature in the workpiece by 49.8%, and average temperature by 17.1 %, indicating a strong influence. At the same time, useful flow rate decreased 3.2 times.

These results indicate that the density is very influential physical parameters of a metalworking fluid.

3.2.6.6 Influence of Surface Tension on the Useful Flowrate and Temperatures

This fluid phenomenon arises from cohesive forces that act between liquid molecules. It is responsible for wetting of solid surfaces and breakup of jets into droplets.

The following grinding setup was used: Wheel diameter = 370 mm, wheel width = 50 mm, grinding depth = 1 mm, nozzle diameter = 6 mm, wheel speed: 20.8 m/s, jet speed: 7.51 m/s, heat generation in the contact zone: $10^{10}$ W/m$^3$. The fluid used in numerical simulation is water, with viscosity that linearly depends on temperature: 0.001002 Pa·s at 20$^\circ$ C, and 0.000282 Pa·s at 100$^\circ$ C. Viscosities out of that temperature range are linearly extrapolated. Figures 3-63 and 3-64 show influence of metalworking fluid surface tension on average and maximum temperatures in the workpiece and the useful flowrate.
Figure 3-63: Average and Maximum Temperatures on the Workpiece vs. Surface Tension of Metalworking Fluid.

Figure 3-64: Useful Flowrate vs. Surface Tension of Metalworking Fluid.
Again, the study was performed over a wide range of values, and shows that the 3 times decrease of surface tension value resulted in 1.42% increase in maximum workpiece temperature and only 0.33% of increase in average temperature. Useful flowrate decreased by 0.7%. An increased surface tension makes metalworking fluid jet more resistant to breakup and increases wetting of the wheel and workpiece surfaces, thus improving the amount of liquid that enters the contact zone, but the effect is not large. The study conforms to the conclusions made by analysis of Weber number of the flow in the section 2.3.3.

3.2.6.7 Influence of Viscosity on the Useful Flowrate and Temperatures

In order to study influence of oils with different viscosity on temperatures in the workpiece and useful flowrates three different oils were chosen with following physical properties:

1) Fluid 1: dynamic viscosity: $\mu$ (at 40°C) = 0.067 Pa·s, $\mu$ (at 100°C) = 0.0056 Pa·s; density: $\rho$ = 890 kg/m$^3$; specific heat: $c_p$ = 2000 J/kg/K; heat conductivity: $k$ = 0.145 W/m/K

2) Fluid 2: dynamic viscosity: $\mu$ (at 40°C) = 0.150 Pa·s, $\mu$ (at 100°C) = 0.0125 Pa·s; density: $\rho$ = 890 kg/m$^3$; specific heat: $c_p$ = 2000 J/kg/K; heat conductivity: $k$ = 0.145 W/m/K

3) Fluid 3: dynamic viscosity: $\mu$ (at 40°C) = 0.220 Pa·s, $\mu$ (at 100°C) = 0.0163 Pa·s; density: $\rho$ = 890 kg/m$^3$; specific heat: $c_p$ = 2000 J/kg/K; heat conductivity: $k$ = 0.145 W/m/K

In figures 3-65 influence of three oils with different viscosity on average and maximum temperatures on the workpiece is presented for three different wheel speeds.

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Figure 3-65: Average and Maximum Temperatures on the Workpiece vs. Metalworking Fluids with Different Viscosities for Different Wheel Speeds.

The results show that if a higher viscosity fluid is used, both average and maximum temperatures decrease. The decrease is more pronounced in values of average temperature. The similar is with different wheel velocities – temperatures of workpiece decrease if the wheel velocity is higher. The higher velocity wheel brings more fluid into
the grinding region (as confirmed in results presented in Fig. 3-66), thus increasing the cooling effect. On the other hand, a low viscosity fluid is desirable in the grinding region in order to decrease frictional losses. Therefore, a desirable fluid would have to be of a non-Newtonian shear thinning type (in the zone from inlet nozzle to the grinding region there is a low shear rate, so viscosity would stay high, but as fluid enters the grinding zone in which shear rates are much larger, the viscosity would decrease).

In figure 3-66 influence of oils with different viscosity on useful flowrate is presented for three different wheel speeds.

![Graph showing useful flowrates for different fluid types and wheel speeds.](image)

Figure 3-66: Useful Flowrates vs. Metalworking Fluids With Different Viscosities for Different Wheel Speeds.
The results in the Fig. 3-66 show that application of fluids with higher viscosities results in higher useful flowrate. The reason for that is probably due to the fact that jets of lower viscosity fluids break up more easily. Therefore, when the jet impacts the wheel and the grinding zone, more fluid is deflected to the sides, thus decreasing the amount of the fluid that enters the grinding zone (useful flowrate).

3.2.6.8 Energy Input Influence on Temperatures in the Workpiece

For this study, 3-D model 2 geometry 1 was extended in order to include the workpiece.

Figure 3-67 shows the outline of the workpiece geometry and two reference cross-section planes generated in order to capture temperature distributions. Only the workpiece is shown, for visual clarity reasons (the other parts of the domain, such as wheel or shield would obstruct the view). Figure 3-68 shows the details of the grid used in the workpiece.
A set of simulation parameters for this study was established. Jet nozzle velocity was 7.51 m/s for all cases, and wheel speed was 20.4 m/s. Energy generation input ranged from 2 W/mm² to 20 W/mm² with 2 W/mm² increment from one case to the next. The
workpiece is not moving. Boundary conditions for the sides of the workpiece were specified as convection boundary conditions with heat transfer coefficient of 20 W/m$^2$/K (in the range of free convection in air), and ambient temperature of 300 K.

Figures 3-69 to 3-88 show contours of temperature in two created cross-section planes – “vertical cross-section plane” and “horizontal cross section plane” for different energy generation inputs.
Figure 3-69: Temperature Distribution in the Vertical Cross-section Plane for Energy Generation of 2 W/mm².

Figure 3-70: Temperature Distribution in the Horizontal Cross-section Plane for Energy Generation of 2 W/mm².
Figure 3-71: Temperature Distribution in the Vertical Cross-section Plane for Energy Generation of 4 W/mm².

Figure 3-72: Temperature Distribution in the Horizontal Cross-section Plane for Energy Generation of 4 W/mm².
Figure 3-73: Temperature Distribution in the Vertical Cross-section Plane for Energy Generation of 6 W/mm².

Figure 3-74: Temperature Distribution in the Horizontal Cross-section Plane for Energy Generation of 6 W/mm².
Figure 3-75: Temperature Distribution in the Vertical Cross-section Plane for Energy Generation of 8 W/mm$^2$.

Figure 3-76: Temperature Distribution in the Hotizontal Cross-section Plane for Energy Generation of 8 W/mm$^2$. 
Figure 3-77: Temperature Distribution in the Vertical Cross-section Plane for Energy Generation of 10 W/mm$^2$.

Figure 3-78: Temperature Distribution in the Horizontal Cross-section Plane for Energy Generation of 10 W/mm$^2$. 
Figure 3-79: Temperature Distribution in the Vertical Cross-section Plane for Energy Generation of 12 W/mm².

Figure 3-80: Temperature Distribution in the Horizontal Cross-section Plane for Energy Generation of 12 W/mm².
Figure 3-81: Temperature Distribution in the Vertical Cross-section Plane for Energy Generation of 14 W/mm².

Figure 3-82: Temperature Distribution in the Horizontal Cross-section Plane for Energy Generation of 14 W/mm².
Figure 3-83: Temperature Distribution in the Vertical Cross-section Plane for Energy Generation of 16 W/mm².

Figure 3-84: Temperature Distribution in the Horizontal Cross-section Plane for Energy Generation of 16 W/mm².
Figure 3-85: Temperature Distribution in the Vertical Cross-section Plane for Energy Generation of 18 W/mm².

Figure 3-86: Temperature Distribution in the Horizontal Cross-section Plane for Energy Generation of 18 W/mm².
Figure 3-87: Temperature Distribution in the Vertical Cross-section Plane for Energy Generation of 20 W/mm².

Figure 3-88: Temperature Distribution in the Horizontal Cross-section Plane for Energy Generation of 20 W/mm².
In order to more closely illustrate differences in temperature fields in cases with different energy generation inputs, Figures 3-89 and 3-90 are presented.

Figure 3-89: Comparison of Temperature Distribution [K] in the Vertical Cross-section Plane for Energy Generation of a) 2 W/mm², b) 6 W/mm².
Figure 3-90: Comparison of Temperature Distribution in the Horizontal Cross-section Plane for Energy Generation of a) 2 W/mm², b) 6 W/mm².

Figures 3-89 and 3-90 clearly indicate that with increased energy generation input the regions of high temperature spread in both vertical and horizontal directions.
Complete results for maximum and average temperatures in the workpiece as a function of heat generation input are shown in Figure 3-91. It can be seen that both maximum and average temperatures are approximately linear functions of heat generation input, but the average temperature curve has a lower slope. The linearity of the curves is result of the linearity of the heat conduction equation, and used constant heat conductivity of the workpiece material.

Figure 3-91: Temperatures in the Workpiece, as a Function of Energy Generation Input.
The presented results came from simulations with motionless workpiece. In order to determine importance of workpiece motion on temperature field, simulations with moving workpiece were performed as well.

In solid regions, the energy transport equation is as follows [10]:

$$\frac{\partial}{\partial t} (\rho \cdot h) + \nabla \cdot (\bar{v} \cdot \rho \cdot h) = \nabla \cdot (k \cdot \nabla T) + S_h,$$

(3.14)

where:

- $\rho$ is density of the material the solid is made of
- $h$ is the sensible enthalpy
- $\bar{v}$ is the velocity of the solid
- $k$ is the heat conductivity of the solid material
- $T$ is the absolute temperature
- $S_h$ is the volumetric heat source.

Equation (3.14) contains a term that represents the influence of energy transfer due to translational motion of the solid region (workpiece). That term is the second term on the left-hand side of the equation.

The x-velocity of workpiece was set to 0.25 m/s that is in the recommended range for aluminum grinding [16]. To illustrate obtained results, Figures 3-92 to 3-95 show temperature fields of cases with, and without workpiece motion for two different heat generation inputs. It can be observed that the left side of the workpiece is warmer in the
case of moving workpiece, because it represents previously grinded region where heat input was present at the time.

Figure 3-92: Temperature Contours in the Vertical Cross-section Plane for Heat Generation Input of 4 W/mm²: a) Workpiece is Stationary, b) Workpiece Moves.
Figure 3-93: Temperature Contours in the Horizontal Cross-section Plane for Heat Generation Input of 4 W/mm²: a) Workpiece is Stationary, b) Workpiece Moves.
Figure 3-94: Temperature contours in the vertical reference plane for heat generation inputs of 20 W/mm²: a) workpiece is stationary, b) workpiece moves.
Figure 3-95: Temperature contours in the vertical reference plane for heat generation inputs of 20 W/mm$^2$: a) workpiece is stationary, b) workpiece moves.
The results are shown in Table 3.17.

Table 3.17: Temperatures on the workpiece for different heat generation and motion inputs.

<table>
<thead>
<tr>
<th>Heat generation</th>
<th>Heat generation</th>
<th>Heat generation</th>
<th>Heat generation</th>
</tr>
</thead>
<tbody>
<tr>
<td>input of 4 W/mm², motionless workpiece</td>
<td>input of 4 W/mm², moving workpiece</td>
<td>input of 20 W/mm², motionless workpiece</td>
<td>input of 4 W/mm², moving workpiece</td>
</tr>
<tr>
<td>Average temperature on the workpiece [K]</td>
<td>311</td>
<td>310</td>
<td>360</td>
</tr>
<tr>
<td>Maximum temperature on the workpiece [K]</td>
<td>367</td>
<td>324</td>
<td>633</td>
</tr>
</tbody>
</table>
From the computed data, the conclusion is that motion of workpiece is more significant in changing the temperature field and average and maximum values for cases when heat generation input is larger. Namely, differences were:

- Maximum temperature difference for case of 4 W/mm² heat generation input: 11.7%
- Maximum temperature difference for case of 20 W/mm² heat generation input: 33.5%
- Average temperature difference for case of 4 W/mm² heat generation input: 0.32%
- Average temperature difference for case of 20 W/mm² heat generation input: 3.05%

A phenomenon of temperature field “smearing” in horizontal cross-section plane in cases of moving workpiece is observed, i.e. temperature field becomes very homogeneous compared to cases when workpiece is stationary.

3.2.6.9 Energy Input Influence on Temperatures of Chip Particles and Temperatures of Workpiece

Grinding process results in removal of some amount of the workpiece. That removed material is called chip. The chip formation was modeled as injection of solid particles.
The size of those solid particles was the same as average chip size which can be analyzed based on volume consistency with removal rate [1]:

\[ V_{cu} = \frac{a_c \cdot v_w}{C \cdot v_s}, \]  

(3.19)

where:

- \( a_c \) is grinding depth
- \( v_w \) is velocity of the wheel
- \( v_s \) is the velocity of the workpiece.

The material removal rate in kg/s was modeled as particle injection mass flowrate [1]:

\[ m = \rho \cdot b_w \cdot a_c \cdot v_w \]  

(3.20)

Where \( b_w \) is the width of the wheel.

For the simulation performed, values used are shown in Table 3.18.

Table 3.18: Parameter values for calculating particle injection flowrate

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho ) = density of aluminum [kg/m³]</td>
<td>2700</td>
</tr>
<tr>
<td>( b_w ) = grinding zone width [m]</td>
<td>0.05</td>
</tr>
<tr>
<td>( a_c ) = grinding depth [m]</td>
<td>0.001</td>
</tr>
<tr>
<td>( v_w ) = grinding wheel velocity [m/s]</td>
<td>65</td>
</tr>
</tbody>
</table>
Using Eq. (3.20), the particle injection massflowrate input was calculated to be 0.008775 kg/s.

The injection position was distributed in the porous region, based on average number of contacts between wheel grains and workpiece surface.

Because some of the heat generated goes into the chip, injected solid particles was described as having temperature and mass. That amount of energy can be calculated using the equation [1]:

\[ \dot{e}_{ch} = \dot{m} \cdot c_W \cdot (T_{ch} - T_{ambient}), \]

(3.21)

Where:

- \( c_W \) is heat capacity of workpiece material.
- \( T_{ch} \) is chip temperature
- \( T_{ambient} \) is the ambient temperature.

Chip temperature \( T_{ch} \) is estimated to be close to melting point of workpiece material, according to [51]. The melting temperature of aluminum is 933 K, so chip temperature was assumed to be 900 K. 3-D Model 2 Geometry 1 was used to do simulations.

Figures 3-96 to 3-103 show some representative results from simulations performed for energy generation of \( 6 \times 10^8 \frac{W}{m^3} \).
Figure 3-96: Chip particles colored by ambient temperature [K].

Figure 3-97: Side view of chip particles colored by ambient temperature [K].
Figure 3-98: Chip particles colored by particle temperature [K].

Figure 3-99: Side view of chip particles colored by particle temperature [K]

In figures 3-98 and 3-99 it can be observed that hot particles, after being injected into the grinding region, get into the contact with the cooler surrounding fluid (Figures 3-96 and 3-97) and quickly assume the ambient fluid temperature as they approach the exit of
the computational domain. Another observation is that the chip particle temperatures are larger close to the side of grinding region.

The particle trajectory pattern shows that there is no accumulation of the chip in the grinding zone or any other part of the domain. Therefore, chip is effectively removed from the domain by the fluid.

Figure 3-100: Chip particles colored by particle temperature [K]
Figure 3-101: Velocity vectors colored by mixture temperature [K]

Figure 3-102: Velocity vectors colored by liquid volume fraction.
In Figures 3-100 and 3-101 the influence of the flow eddies on the injected particle trajectory is evident. Swirling of the surrounding fluid deflects the particles and causes convergence of their trajectories in several places.

A parametric study of particle injection influence on temperatures was performed with following setup:

- Nozzle jet velocity = 60 m/s
- Wheel velocity = 65 m/s
- Initial particle temperature: 900 K
- Particle injection mass flowrate: 0.008775 kg/s
- Energy generation input (particle energy not included): $3 \cdot 10^8$, $6 \cdot 10^8$, $9 \cdot 10^8$, $12 \cdot 10^8$ and $15 \cdot 10^8$ W/m$^3$

Injected particles accounted up to 65 to 90 % of the total energy generation input.
Figure 3-104 shows results of simulations.

Figure 3-104: Temperature of injected particles and temperatures on the workpiece

The curve of maximum workpiece temperatures shows similar nonlinearity to curves shown on Figure 3-32. Average temperature of the workpiece linearly rises with increasing heat generation rate, but minimum particle temperature shows a much modest increase in temperature. The maximum temperature (the same as the initial particle temperature as they are injected into the grinding region) of the particles is not shown, and is assumed to be 900 K in all cases.
3.3 2-D model

3-D simulations are normally required in order to get realistic fluid flow and temperature fields and the most accurate data possible. However, 3-D computations can entail high computational and time resources. For practical reasons, a 2-D model may be more valuable, even though, a loss of accuracy can be expected. For example, a typical 2-D Model case was solved in about one hour, compared to a typical 3-D Model 2 case that took about 70 hours to converge. Simulations were performed on a workstation PC with 12 GB of RAM and Intel i7 Xeon four-core processor at 3.066 GHz. Some main features of the 2-D model, including an example work parameters, are shown in the following sections.

3.3.1 Geometry

The Figure 3-105 shows some of the most important parts of the 2-D Model’s geometry such as: grinding wheel (diameter is 260 mm), metalworking fluid inlet, the shield, porous grinding region and workpiece. These parts are the same like in 3-D Model 2.
Figure 3-105: Outline of 2-D model
3.3.2 Grid Properties

Table 3.19: 2-D Model Grid Quality.

<table>
<thead>
<tr>
<th>Minimum Orthogonal Quality</th>
<th>0.664440</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum Aspect Ratio</td>
<td>2.52683</td>
</tr>
</tbody>
</table>

Table 3.20: 2-D Model Grid Size

<table>
<thead>
<tr>
<th>Cells</th>
<th>36549</th>
</tr>
</thead>
<tbody>
<tr>
<td>Faces</td>
<td>74449</td>
</tr>
<tr>
<td>Nodes</td>
<td>37897</td>
</tr>
<tr>
<td>Partitions</td>
<td>1</td>
</tr>
<tr>
<td>Cell zones</td>
<td>2</td>
</tr>
<tr>
<td>Face zones</td>
<td>17</td>
</tr>
</tbody>
</table>

Compared to the 3-D Model 1 Geometry 1, it can be seen that the number of cells in 2-D Model decreased by a factor of about 56.
Figures 3-106 and 3-107 show details of the grid for the 2-D Model.

Figure 3-106: Grid for 2-D Model.
The Fig. 3-107 shows the grid of grinding region in detail. It can be seen that it is much finer than the grid used for the other domains in order to correctly capture flow features.

3.3.3 Numerical Setup and Physics

Table 3-21 shows the most important numerical parameters and physical models chosen for the simulations using 2-D Model. The same setup was used as in 3-D Model 2.
Table 3-21: Numerical and physical setup

<table>
<thead>
<tr>
<th><strong>Solver type:</strong></th>
<th>Pressure based 2D double precision</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Simulation type:</strong></td>
<td>Steady state calculations</td>
</tr>
<tr>
<td><strong>Velocity formulation:</strong></td>
<td>Absolute</td>
</tr>
<tr>
<td><strong>Gradient option:</strong></td>
<td>Green-Gauss Cell Based [18]</td>
</tr>
<tr>
<td><strong>Turbulence model:</strong></td>
<td>Reynolds Stress Model [19]</td>
</tr>
<tr>
<td><strong>Multiphase model:</strong></td>
<td>Volume of Fluid (VOF) 2-phase model</td>
</tr>
<tr>
<td></td>
<td>(liquid and gas), which includes surface tension and wall adhesion</td>
</tr>
<tr>
<td><strong>Momentum, turbulent kinetic energy, turbulent dissipation rate, Reynolds stresses and energy equation discretization method:</strong></td>
<td>Third order MUSCL [20]</td>
</tr>
<tr>
<td><strong>Pressure discretization method:</strong></td>
<td>Body-force weighted</td>
</tr>
<tr>
<td><strong>VOF discretization method:</strong></td>
<td>High Resolution Interface Capturing [21]</td>
</tr>
<tr>
<td><strong>Porous zone motion:</strong></td>
<td>Rotating reference frame</td>
</tr>
<tr>
<td><strong>Pressure-velocity coupling:</strong></td>
<td>Phase coupled SIMPLE [22]</td>
</tr>
<tr>
<td><strong>Residual absolute criteria:</strong></td>
<td>$10^{-6}$ for energy and $10^{-3}$ for velocities, $k$, $\varepsilon$, water volume fraction and continuity</td>
</tr>
<tr>
<td><strong>Grinding zone porosity:</strong></td>
<td>50%</td>
</tr>
</tbody>
</table>
3.3.4 Numerical and Experimental Validations

A validation of 2-D model was performed, by comparing the results of 2-D Model with results of 3-D Model 2 Geometry 1 and experimental data. The comparison is shown in Figures 3-108 and 3-109. 2-D simulations yielded larger percentage of useful flow rate because of inability of the fluid to move sideways to the wheel when hitting the grinding zone and grinding wheel. The average error for 2-D simulations is 34% compared to 13% for 3-D simulations, the trend of curves is similar, but 3-D simulation results are closer to experimental values for higher nozzle jet velocities.

Figure 3-108: Useful Flow Rate Percentage Comparison for 2-D and 3-D Simulations and Experiments
To numerically validate the model, a grid dependence study was performed with following parameters: coarser mesh: 36549 cells, finer mesh: 68843 cells. The average difference in useful flowrate for different nozzle flow rates for those two different grids was about 0.5 %. The results are shown in Fig. 3-110.
3.3.5 2-D Model Results

A set of parametric studies was performed to analyze the influence of different input parameters on fluid flow and heat transfer in and around grinding area. Chosen parameters were: nozzle angle, fluid flow rate and type of grinding fluid. The geometrical characteristics of the model were kept the same: wheel diameter = 260 mm, grinding depth = 1 mm, workpiece thickness = 28 mm, distance from the nozzle to the grinding zone = 150 mm, circumferential wheel velocity = 50 m/s.
3.3.5.1 Influence of the Nozzle Angle on the Useful Flowrate and Temperatures

Figure 3-111 shows results for the influence of different jet nozzle angles on useful fluid flow rate. Nozzle angle is measured from the horizontal with positive values in downward direction. It can be seen that the dependence function is a convex curve with a maximum at about 10 degrees. This angle value corresponds to tangential delivery of grinding fluid to the grinding zone.

![Graph showing useful flow rate vs. nozzle angle]

Figure 3-111: Useful Flow Rate vs. Nozzle Angle.

The impact of the jet nozzle angle on the maximum temperature on the work piece is graphically presented in figure 3-112. The function has a minimum at about 10 degrees, which corresponds to the position of maximum useful flow rate in the figure 3-111 (larger amounts of useful flowrate help in cooling).
Figure 3-112: Maximum Temperature on the Work Piece vs. Nozzle Angle.

Figures 3-113 to 3-115 show vectors of grinding fluid velocity in the area between fluid inlet and the grinding region for different jet angles (0, 10 and 30 degrees respectively). It can be seen that the flow field is quite different for different jet angles. The part of the inlet jet that reverses the direction of flow (due to the contact with the wheel) decreases in height when nozzle angle is increased. Figure 3-116 shows velocity vectors in zoomed grinding region.
Figure 3-113: Velocity Vectors for 0 Degree Jet Angle.

Figure 3-114: Velocity Vectors for 10 Degree Jet Angle
Figure 3-115: Velocity Vectors for 30 Degree Jet Angle

Figure 3-116: Velocity Vectors in Grinding Region.
3.3.5.2 Influence of Nozzle Flowrate on the Useful Flowrate and Temperatures

Figures 3-117 and 3-118 shows the useful flow rate and maximum temperature on the work piece as functions of the nozzle mass flow rates. Other geometrical and process parameters were the same as in simulations regarding the nozzle angle. Nozzle angle was set to 10 degrees. Results show that the maximum temperature on the part decreases as the fluid flow rate increases. A larger fluid supply has greater cooling potential thus lowering temperatures in the work piece. However, as the flow rate is increased, the cooling effect is less pronounced, showing a saturation effect (similar to 3-D simulations presented in Fig. 3-44).

![Figure 3-117: Useful Fluid Flow Rate Percentage](image_url)
3.3.5.3 Influence of grinding fluid type

The two types of fluids considered were water and oil, which have different physical characteristics such as: density, viscosity, heat capacity, surface tension and thermal conductivity. The properties considered are presented in Table 3.22, and they were assumed to be constant. However, the model is general and can include variations of those properties with temperature.
Table 3.22: Physical Properties of Oil and Water.

<table>
<thead>
<tr>
<th>Fluid type</th>
<th>Oil</th>
<th>Water</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density [kg/m$^3$]</td>
<td>873</td>
<td>998</td>
</tr>
<tr>
<td>Specific heat capacity [J/kg/k]</td>
<td>1670</td>
<td>4182</td>
</tr>
<tr>
<td>Thermal conductivity [W/m/K]</td>
<td>0.12</td>
<td>0.6</td>
</tr>
<tr>
<td>Viscosity [kg/m/s]</td>
<td>0.02</td>
<td>0.001003</td>
</tr>
<tr>
<td>Surface tension [N/m]</td>
<td>0.025</td>
<td>0.075</td>
</tr>
</tbody>
</table>

Grinding parameters were kept the same for both simulations: wheel diameter = 260 mm, grinding depth = 1 mm, work piece thickness = 28 mm, distance from the nozzle to the grinding zone = 150 mm, fluid velocity at the nozzle = 50 m/s, circumferential wheel velocity = 50 m/s.

Figures 3-119 and 3-120 show temperature fields in work piece for simulations with oil (Figure 3-119) and water (Figure 3-120). It is clear that water based fluid provides better cooling due to higher specific heat capacity and thermal conductivity (in Table 3.23 the maximum temperatures are shown). The right hand side part of the workpiece is cooler than the left hand side due to the contact with the cool fluid it comes into contact with.
Figure 3-119: Temperature Distribution in Work Piece for Oil as the Grinding Fluid [K].

Figure 3-120: Temperature Distribution in Work Piece for Water as the Grinding Fluid [K].
Use of different grinding fluids not only changes the temperature field distribution, but the velocity field as well. This effect is well observed in Figures 3-121 and 3-122. The reason for this difference lies in different properties of water and oil such as density, viscosity and surface tension.

Figure 3-121: Velocity Vectors for Case with Oil as Grinding Fluid [m/s].
Figure 3-122: Velocity Vectors for Case with Water as Grinding Fluid [m/s].

Figures 3-123 and 3-124 show velocity vectors of oil and water in the zoomed grinding region. The colors indicate that a larger volume fraction of liquid is present in the grinding zone in the case when water was used, compared to the case with oil as metalworking fluid.
Figure 3-123: Velocity Vectors in Grinding Region for Oil Colored by the Volume Fraction of Oil.

Figure 3-124: Velocity Vectors in Grinding Region for Water Colored by Volume Fraction of Water.
The data regarding percentage of useful flow rate and maximum temperature on the workpiece from simulations with oil and water is presented in Table 3.23.

Table 3.23: Simulation Results for Different Types of Grinding Fluid.

<table>
<thead>
<tr>
<th>Fluid type</th>
<th>Oil</th>
<th>Water</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum temperature of the workpiece [K]</td>
<td>805</td>
<td>421</td>
</tr>
<tr>
<td>Percentage of useful flowrate</td>
<td>19.64</td>
<td>23.62</td>
</tr>
</tbody>
</table>
Chapter Four

Conclusions and Future Work

The simulations performed proved the feasibility of the CFD multiphase flow and heat transfer simulations in grinding. Three different models were built: 1) global fluid flow 3-D Model 1 which was used to analyze the whole flow geometry and capture significant boundary conditions for the second model, 2) detailed 3-D Model 2 of the grinding zone and its vicinity with complex fluid and solid physical properties used to analyze fluid flow rates, temperatures and pressures, and 3) 2-D Model used to study influence of fluid and fluid delivery parameters on temperatures and useful flowrate. The models were validated both numerically and by comparing to experimental data found in recent literature. The chosen porosity models were proven as adequate. Useful information and realistic fluid behavior were obtained. The results for useful flow rates and temperatures occurring in the grinding region matched results found in literature with good precision and conformability. Distributions of temperatures, pressures and flow rates in and around grinding region were obtained in great detail, which would be difficult or even impossible to obtain using experiments only. These results are essential in studying and understanding the influence of the fluid on the parameters and outcomes of a grinding
process, as well as in determining the best fluid composition and supply parameters for a given application.

The behavior of two different multiphase models was investigated. Results indicated that VOF model outperformed Eulerian model, especially at high wheel velocities.

Performances of three different turbulence models were investigated: realizable k-epsilon, SST k-omega and Reynolds stress model. Results showed that Reynolds stress model yielded the most accurate results over a wide range of wheel and jet velocities, while k-epsilon, and especially k-omega model tended to overpredict the useful flow rate. More accurate performance of Reynolds stress model can be attributed to superior Reynolds stress transport model versus Boussinesq approach used in k-epsilon and k-omega models.

A set of parametric studies was performed using 3-D Model 2 in order to analyze influence of different fluid properties on useful flowrates and temperatures. The following conclusions can be made:

- The influence of specific heat is not negligible and was more significant on the temperatures in the workpiece than the useful flowrate
- Due to very small changes in temperatures in the workpiece and useful flowrate for cases with large differences in heat conductivity, the conclusion is that k cannot be used as an effective property to control the temperature distribution in the grinding region
- The results for the density study showed that density is very influential physical parameter of a metalworking fluid, particularly on the temperatures developed in the grinding region
• An increased surface tension makes metalworking fluid jet more resistant to breakup and increases wetting of the wheel and workpiece surfaces, thus improving the amount of liquid that enters the contact zone, but the effect is quite small.

• The results show that if a higher viscosity fluid is used, both average and maximum temperatures decrease. The decrease is more pronounced in values of average temperature; a desirable metalworking fluid would have to be of changing viscosity in order to perform well in different parts of the flow (high viscosity in the zone from nozzle to the grinding region, and low viscosity in the grinding region itself).

• The results for maximum and average temperatures in the workpiece as a function of heat generation input show that both maximum and average temperatures are approximately linear functions of heat generation input, but the average temperature curve has a lower slope; the linearity of the curves is result of the linearity of the heat conduction equation, and used constant heat conductivity of the workpiece material.

• A study of influence of workpiece motion on temperatures was conducted, as well; from the computed data, the conclusion is that motion of workpiece is more significant in changing the temperature field and average and maximum values for cases when heat generation input is larger.

• Chip formation was modeled as particle injection and a study was performed to observe influence of heat generation input on temperatures in the grinding zone; injected particles quickly assumed the ambient fluid temperature as they...
approached the exit of the computational domain; another conclusion is that the chip particle temperatures were larger close to the side of grinding region; the particle trajectory pattern showed that there was no accumulation of the chip in the grinding zone or any other part of the domain, therefore, chip is effectively removed from the domain by the fluid.

2-D Model was used to perform parametric studies of influence of metalworking fluid flow delivery and type influence on temperatures and useful flowrates. The following conclusions can be made:

- The data on influence of nozzle angle on useful flowrate showed that dependence function is a convex curve with a maximum at about 10 degrees of nozzle angle; this angle value corresponded to tangential delivery of grinding fluid to the grinding zone; maximum temperature curve had minimum at 10 degrees of nozzle angle, as well, because larger amounts of metalworking fluid help in cooling.

- A study of the dependence of useful flowrates and maximum temperature on the workpiece on the nozzle mass flowrates showed: 1) the useful flowrate percentage graph is a convex curve, with a maximum at a particular value of nozzle jet flowrate, 2) maximum temperature on the part decreased as the fluid flow rate increased.

- The performance of two types of metalworking fluids considered were water and oil, which have different physical characteristics such as: density, viscosity, heat capacity, surface tension and thermal conductivity; it was obvious that water based fluid provided better cooling due to higher specific heat capacity and thermal conductivity; use of different metalworking fluids not only changed the
temperature field distribution, but the velocity field as well; another conclusion was that a larger volume fraction of liquid was present in the grinding zone in the case when water was used, compared to the case with oil as metalworking fluid.

The future development of this work can be in several different directions:

- Fluid-structure coupling with solid mechanics chip-removal models in order to simulate the workpiece and wheel deformation and its impact on the fluid flow and heat transfer
- Analysis of performance of different types of non-Newtonian fluids as metalworking fluids
- Analysis of temperature fields in the grinding wheel
- Inclusion of metalworking fluid evaporation and fully porous wheel.

The proposed extensions of this work aim to include more complex models of different mechanical engineering branches in order to make a more holistic approach that would bring simulations even closer to the physical reality of grinding process, enable tool wear and workpiece surface quality evaluation, and further analysis and optimizations.
References


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