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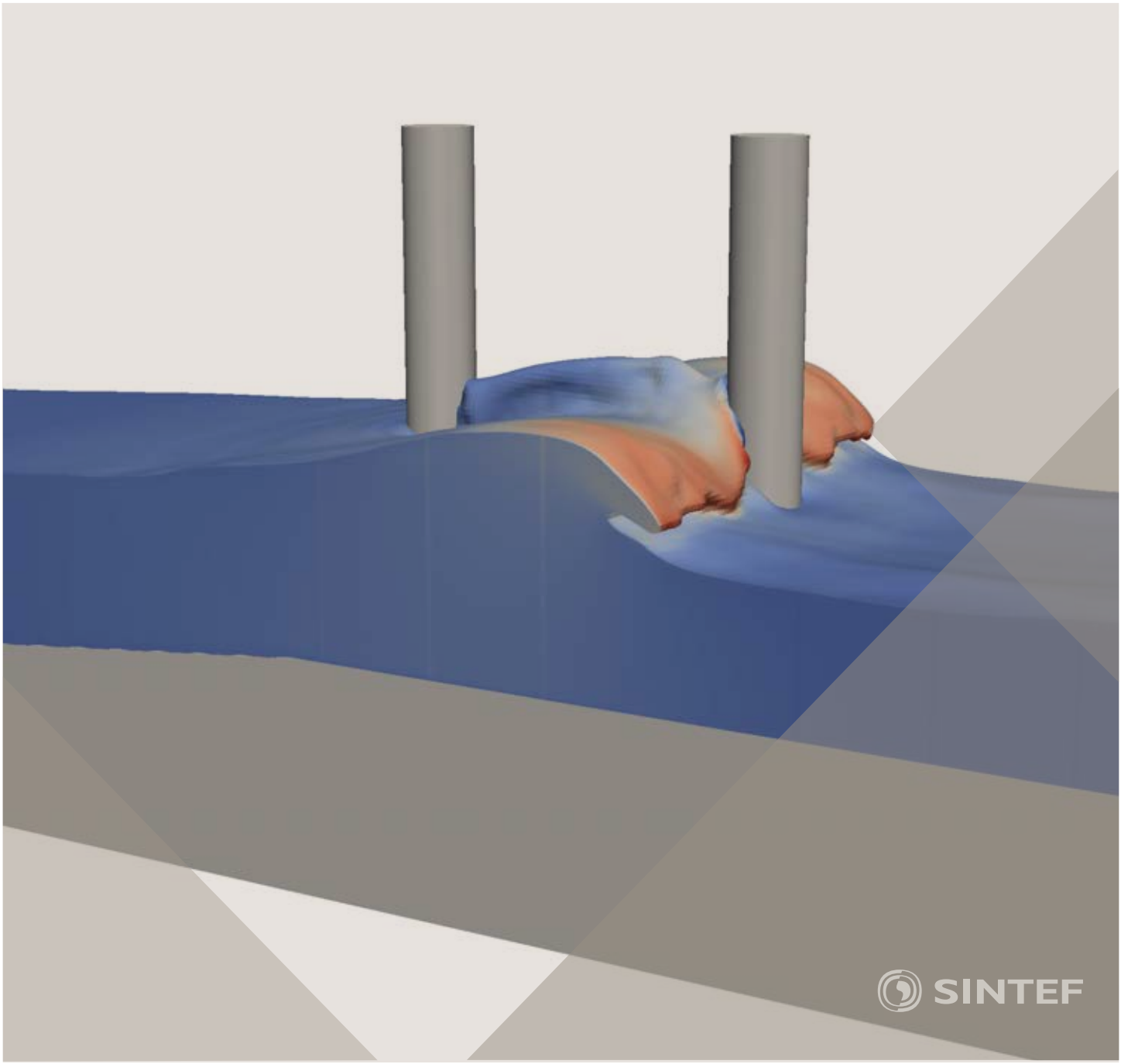
Proceedings of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries

Progress in Applied CFD – CFD2017



SINTEF Proceedings

Editors:
Jan Erik Olsen and Stein Tore Johansen

Progress in Applied CFD – CFD2017

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PREFACE

This book contains all manuscripts approved by the reviewers and the organizing committee of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in May/June 2017 and is also known as CFD2017 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focuses on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. In addition pragmatic modelling concepts and bio-mechanical applications have become an important part of the conference. The papers in this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are included in the proceedings. 108 contributions were presented at the conference together with six keynote presentations. A majority of these contributions are presented by their manuscript in this collection (a few were granted to present without an accompanying manuscript).

The organizing committee would like to thank everyone who has helped with review of manuscripts, all those who helped to promote the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: ANSYS, SFI Metal Production and NanoSim.

Stein Tore Johansen & Jan Erik Olsen

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USE OF CFD AS A DESIGN TOOL FOR A PHOSPHORIC ACID PLANT COOLING POND

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ABSTRACT

Phosphate fertilizer plants are installations constantly evolving which make their design a challenging task. Phosphogypsum, a by-product of the manufacture of phosphoric acid, is piled up, forming stacks which may eventually alter the process efficiency as they encroach on process cooling ponds and locally modify the airflow fields. The easier access to high performance computing and the improvement of software capabilities allow to fully consider today the use of CFD within tight-schedule industrial projects, even the ones involving large-size geometry. As an example we describe how CFD can be efficiently used as a design tool for the revamping of a phosphate fertilizer complex. The use of recently emerged multi-software optimization tool is also explored as a way to enhance the engineering time dedicated to this problem.

Keywords: CFD, Fluid-Fluid interaction, Heat exchange, Optimization, Pollutant dispersion.

NOMENCLATURE

Greek Symbols

α Water mass fraction.

Latin Symbols

V Velocity, [m/s].
T Temperature [°C].
z_0 Roughness length, [m].

Sub/superscripts

a Air.
p Pond

INTRODUCTION

The enhanced accessibility to faster cores has led to an important evolution of high computing performance (HPC) for CFD. In addition, most of the current commercial softwares are now well optimized to take advantage of this available higher power resources, allowing large-size geometry parallelization. This has opened up new opportunities for CFD to be part of industrial projects as a design tool in domains where it was not a conceivable option just a few years ago, due to the incompatibility between the project schedules and the time consuming calculations. Furthermore, CFD studies on the atmospheric boundary layer are now common [DUYNKERKE, 1988] [VENDEL et al, 2010] and allow to model a complete plant subjected to various weather conditions. Based on Pasquill classes [PASQUILL, 1971], different wind velocity, temperature and turbulence profiles can be applied to represent real atmospheric conditions. In Oil & Gas industry, two frequent examples are the Hot Air Recirculation studies performed on Liquefied Natural Gas (LNG) trains and the pollutant dispersion studies around onshore and/or offshore installations [DEVYNCK, 2016]. Another less familiar application involving the modeling of large geometry and for which CFD can be a helpful design option is the phosphate fertilizer plant.

This kind of plant may be associated with several problematics such as fluoride dispersion, steam fog formation or process thermal management. Fluoride is a major pollutant involved in the phosphoric acid production process which usually consists of the reaction between phosphate rock and sulphuric acid (wet process). Its release in the atmosphere from the evaporative cooling pond surface must be carefully monitored to ensure the respect of the regulations. Moreover, the cooling process taking place in the ponds leads to an important increase of the water content in the ambient air, which can cause steam fog formation under unfavourable weather conditions. Whether it is for the dispersion of fluoride or the steam fog formation prediction, not only CFD can allow to assess the situation but also to explore improvement solutions.

Another concern regarding the phosphate fertilizer plants comes from the formation over time of large phosphogypsum stacks which may eventually lead to the necessity to revamp the plant. The phosphogypsum, a by-product of the manufacture of the phosphoric acid during the so called wet process, is mixed with water to form a slurry, then continuously piled up in settling ponds which will turn into massive gypsum stacks after years of service. About 5 tons of phosphogypsum are produced for each ton of phosphoric acid [GOWARIKER et al, 2009]. To allow the gypsum stack expansion, new deposit areas must be defined. The conversion of a cooling pond into a settling pond is then a possible solution even though it leads to the reduction of the heat

exchange surface. As a result, new ways to exchange energy or to reduce the process total heat duty requirement must be found. The easiest way to achieve this may be by revamping the process in order to reduce the total dissipated energy and to optimize the remaining exchange surface. Revamping plants is a quite common task for Oil & Gas engineering companies nowadays and CFD can be used to support the optimization of the remaining pond surface.

MODEL DESCRIPTION

Overall geometry

To account for a phosphate site production, a typical area has been reproduced. It consists in two gypsum stacks whose only one is still active with a settling pond at the top. Three cooling ponds are used on that plant, including one at the top of the non-active gypstack. Surrounding elements such as process units and houses of the residential area have also been modeled (Figure 1). The atmospheric part of the domain is modeled by a box whose dimensions are 2km x 2.5km x 1km.

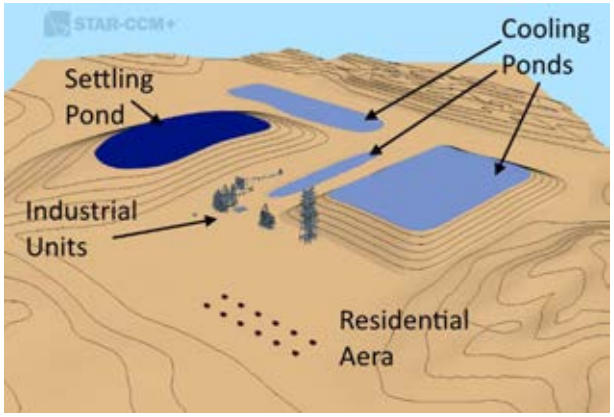


Figure 1: Overall domain

The presence of irregular terrain close to the site can be included into the simulation starting either from 2D elevation lines or directly from a 3D topography surface. Using STAR-CCM+ surface wrapper we reconstructed a CFD compatible ground surface.

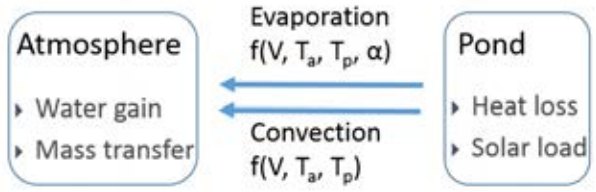
In the following demonstration study, the irregular terrain elevation has been imported as STL files while stacks have been entirely built from the 3D-CAD modeler of STAR-CCM+. All parts of interest for the study must be included in the computational domain in order to take into account the congestion and the air flow disturbance. Moreover, this could also be of importance for controlling precisely the amount of pollutant in the installation area.

A residential area represented by 12 houses has been implemented at about 500 meters of the closest pond. Likewise, process industrial structures are positioned at about 100 m from the pond.

Fluid-Fluid interaction

To account for the evaporation taking place from the pond surface without computing the real gas-liquid interface, we modeled it as a fluid-structure interface. Two independent fluid regions are exchanging data through the interface in order to compute the calibrated heat and mass exchange. Several benefits come from the separation of the two regions: the physics is simplified as there is no more need for multiphase flow modeling. Instead, two single phase flow calculations are performed simultaneously and only an exchange of some specific values at the interface is required. Using data mapping technique with nearest neighbour interpolation, water temperature value is sent to the atmosphere region whereas the calculated evaporative and convective heat fluxes values are transmitted to the pond region to cool down the liquid.

Several field functions accounting for the evaporative and convective heat fluxes and the water mass flow rate at the air/pond interface have been defined. The main local parameters used by the solver to feed those functions are the air velocity, the air temperature, the relative humidity and the water temperature. The different exchanges taking place between the two fluid domains are summarized by the following diagram.



The evaporation correlation is based on daily experimental data measurements over several years and is detailed in § Heat management computations.

Another important advantage arising from the flat interface hypothesis is to allow the use of coarser meshes. Table 1 gives a comparison of the mesh size of two identical domains varying only by the modeling approach (1 fluid region versus 2 fluid regions).

Table 1: Number of cells

	Air	Water	TOTAL
2 regions	184,858	102,090	286,948
1 region	2,240,000	717,066	2,957,142

It is obvious that adopting the two separated fluid zone modeling will allow a significant computational time reduction which is preferable for the purpose of conducting optimization study which can require to perform numerous simulation runs.

Mesh

Due to the large surface and the very small depth of the ponds, the thin mesher technique has been used in the water region. Ten cells have been generated over the water depth to discretise sufficiently the cooling pond. There is no need to use a conformal mesh at the interface due to the employed interpolation technique (§ Fluid-Fluid Interaction). Thus, with a cell size of the same magnitude at both interface sides, yet adopting two

different meshing method for the fluid zones, the final mesh can be coarser while remaining relevant to model the heat exchange and the flow in the two regions.
In the air zone, a trimmed mesh has been used with one prism layer generated on the ground. The ground surface cell size has been set to 5m while a 2m size has been imposed on the pond surface. During the surface wrapping operation, different target sizes have been defined on the structure elements according to the desired level of precision. The minimum cell size allowable has been set to 10 % of the base size.

The Figure 2 shows the differences between the initial faceted surface (STL) and two generated surface meshes set with different base sizes, respectively 5 m and 10 m.

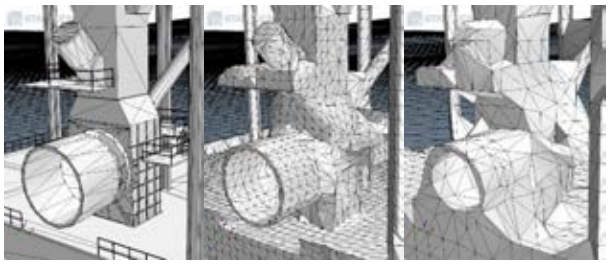


Figure 2: STL file, Wrap 5m, Wrap 10m

Given the potential for the rapid growth of the total cell number, only the areas of interest, such as the air intakes or the areas nearby the workers should be precisely discretised.

Pond Optimization

Following the removal of one of the cooling pond to allow space for the active gypsum stack expansion, a significant surface which was dedicated to the dissipation of the energy is no longer available. Consequently, modifications must be made to the process to recover the lost heat duty, thus ensuring to maintain the process efficiency. In order to achieve this objective, the remaining cooling ponds must be optimized as well to make them the most efficient possible.

On this basis, the second pond which offers the highest potential due to its larger size, has been modeled separately with the purpose to optimize the surface heat exchange. As the overall geometry of the pond cannot be modified, only realistic on-site implementations have been explored such as modification of the water inlets/outlets position and the addition of elements to modify the water distribution, such as dikes.

Figure 3 highlights the CFD study domain which includes only the cooling pond and the non-active gypsum stack to keep the number of cells to a reasonable amount. Indeed, the optimization study can require a lot of calculation runs to determine the global optimum or to plot a Pareto front which helps to determine the feasible designs depending on the defined constraints and objectives.

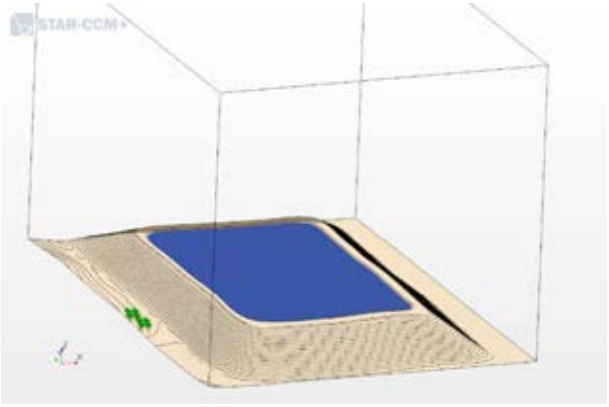


Figure 3: Optimization domain

The optimization tool used for this study is HEEDS which is a multidisciplinary design exploration software from Siemens PLM Software. After the definition of several parameters adjustable by the solver and several target objectives, the selected optimization algorithm will explore the whole space design in order to find local or global optimum. As this exploration process is automated within HEEDS, the final geometry and mesh model must be robust to ensure the good convergence of the different calculations. Consequently, all the standard manual manipulations such as “surface repair” or “diagnostics” are avoided and must be configured to be automatically performed.

In order to modify the water distribution inside the pond, dikes have been created via the 3D-CAD modeler to be added to the pond model. The parameters defined as being modifiable by the software to find the better designs are:

- Number of dikes (from 1 to 10).
- Depth of the pond (from 0.5m to 5m)
- Orientation of the dikes (North-South or East-West)
- Aperture between side of the pond and dikes (20 to 200m)

A JAVA macro is also executed before the start of the simulation in order to modify the position of the water inlet inside the pond. Indeed, depending on the number of dikes and their orientation, the inlet may be located at three different locations, while the outlet remains fixed.

As a finer mesh is required close to the dikes, the total number of cells in the domain will change significantly according to the parameter set configuration. The total number of cells can vary between 300,000 cells and 2,500,000 cells.

Two objectives have been defined: improve the surface heat transfer and reduce the investment costs (CAPEX). On a practical level, this involves the lowest outlet temperature possible while minimizing the dikes length.

Boundary and Operating conditions

Air domain

The atmospheric domain has been set to orient the cell faces perpendicularly to the wind direction. Wind is coming from the east direction with a neutral wind stability profile (Pasquill class D). Wind velocity is 3 m/s at 10 m elevation. The wind temperature is assumed to be constant and equal to 25°C.

The two side faces parallel to the wind direction are considered as symmetry planes, such as the top of the atmospheric box. The last bounding box face has been set as a pressure outlet.

The atmospheric boundary layer has been modeled through the best practices of STAR-CCM+ and the roughness of the ground has been set to represent an agricultural land with some large obstacles by a distance of 500 meters (z_0=0.035).

On the water surface, a slip condition for air has been set. That leads to increase the wind velocity far from the side of the pond. A water mass flux source term has been defined. It depends on the wind velocity, the air temperature, the water content and the water temperature (see § Fluid-Fluid Interaction). Convective and evaporative heat transfer are computed via the correlations explained above. A realizable k-epsilon turbulence model has been used.

Water domain

The pond's bottom and side faces are considered adiabatic with a no-slip condition. The interface is treated like a free surface, i.e with a slip condition and with a thermal heat sink corresponding to the evaporation and the convection heat flux. A realizable k-epsilon turbulence model has been used.

RESULTS

Pollutant dispersion

Fluoride emissions from the ponds may raise concerns if the concentration reaches the regulatory limits. Safety and environmental studies are a large part of all the industrial projects. They aim to ensure the protection of the site workers and the population living in the plant vicinity. It is for this reason that the fluoride released by the eastern stack surface has been studied using a multi-gas approach.

The Figure 4 represents an overhead view of the plant and highlights the fluoride plume expansion. The wind coming from the right face of the atmospheric box (south east direction) drives the pollutant towards the installations and the residential area.

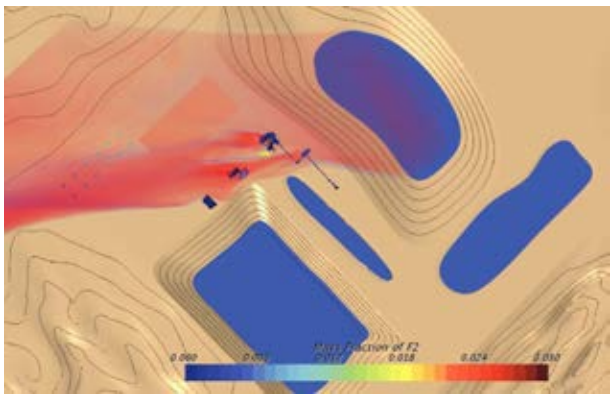


Figure 4: Fluorine plume expansion

The concentration of fluoride can also be displayed on the wall of the area of interest such as the residential area or the process equipment. Due to the discrepancy between the regulatory limits regarding the working area and the residential area (8 hour exposures vs yearly exposure) two scales of concentration must be plotted.
On that example, an 8-hour mass fraction exposure limit of 0.027 (fictional value) of fluoride is drawn in Figure 5 on working area and a yearly mass fraction exposure limit of 0.015 (fictional value) of fluoride on the houses representing the residential area on Figure 6.

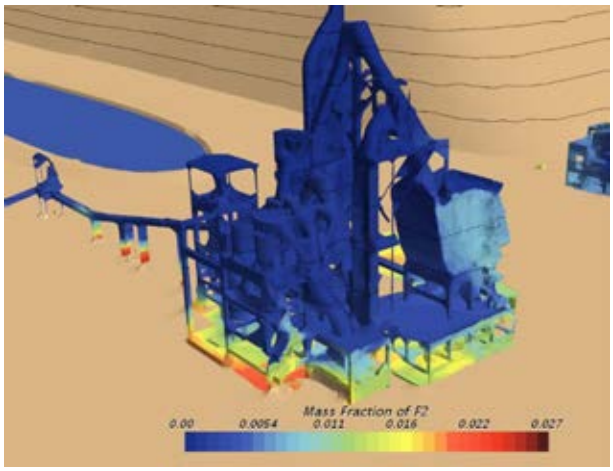


Figure 5: 8Hr exposure limit on working area

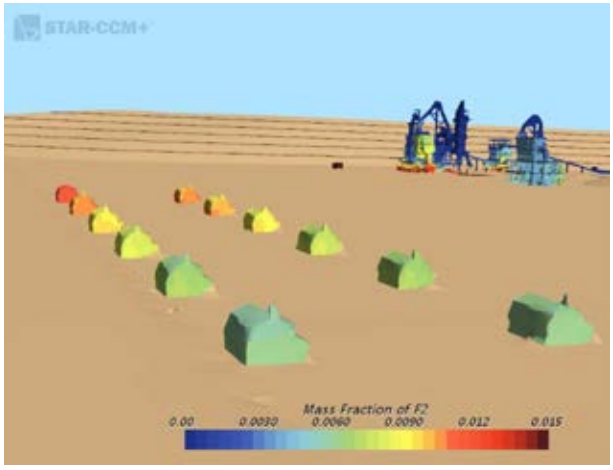


Figure 6: 1yr exposure limit on residential area

Heat management computations

The main role of the cooling ponds is to exchange a large amount of heat with the atmosphere, thus reducing the process water temperature. Any modification of the upstream process (inlet water temperature, water flowrate, etc) or of the cooling pond surface will affect its performances.

Base case

First of all, the active configuration has been modeled and compared to experimental on-site measurements. Three ponds are used to cool the process water, two on the ground level and one at the top of an old gypsum stack.

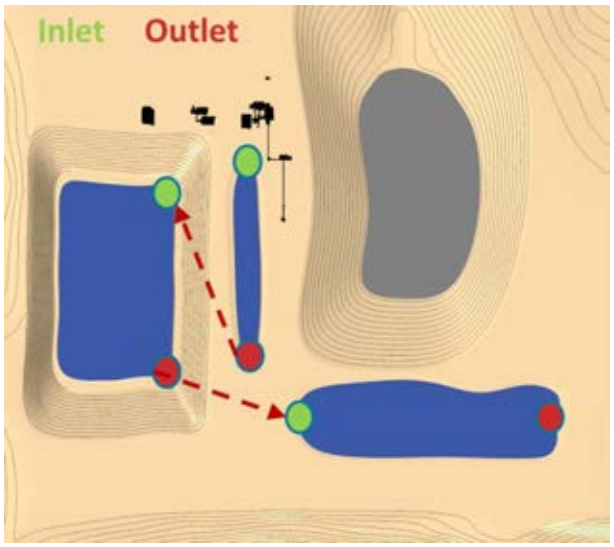


Figure 7: Base case modeling

According to on-site daily measurements, an evaporation correlation has been established depending on wind velocity, air temperature, water content in air (moisture) and water temperature. The way to exchange the values between the water and the air is described in § Fluid-Fluid Interaction. The convective heat transfer has also been taken into account depending on wind velocity, air temperature and water temperature.

Figure 7 represents the running order of the three ponds. The water is entering in the first and smaller pond at 48°C. Figure 8 shows the computed water surface temperature in the different ponds.

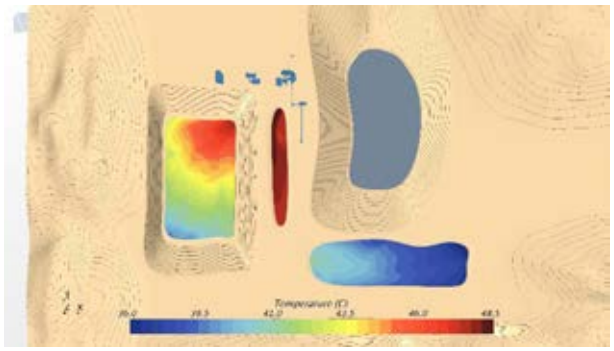


Figure 8: Base case surface temperature

The calculation allowed to highlight the contribution of the last – and soon to be remove - pond to the total heat exchange. Water temperature drops by 4°C in this pond which represents 52 MW (about 30% of total heat exchange).

Pond optimization

All the results extracted from STARCCM+ by HEEDS have been compared to a base case without dikes and a pond depth of 2m (Figure 9). The outlet temperature is 44.43°C and the error margin has been estimated to be 0.2°C (5% of the heat exchange). More than 120 computations have been performed, including less than 15% that have failed due to divergence problems or results inconsistency.

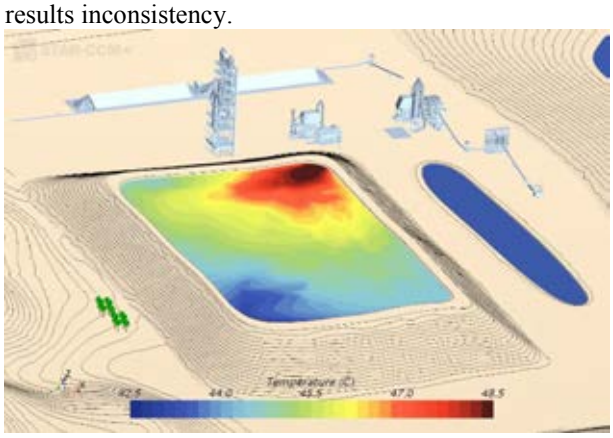


Figure 9: Optimization - No dikes, 2m depth

Some of the optimization results were very close to each other, within the error margin. That led to select not one, but several "best design" and to extract the trends regarding the effects of the different parameters.

As an example, we present two different solution designs leading to an equivalent outlet temperature (Figure 10 and Figure 11):

- 6 horizontal dikes, large opening, small depth
  Outlet temperature = 43.8°C
  Heat duty gain = 15.2%

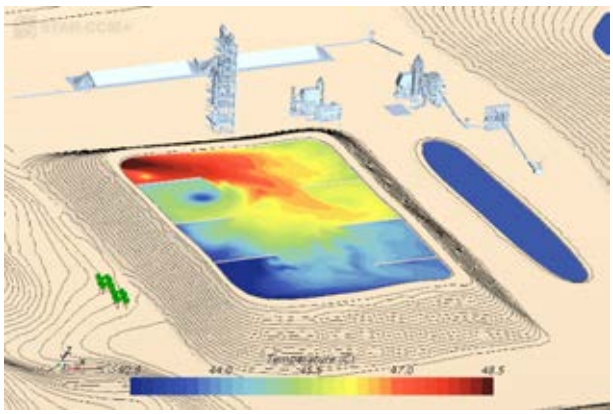


Figure 10: 6 horiz. dikes, large opening, small depth

- 1 horizontal dike, large opening, small depth
  Outlet temperature = 43.65°C
  Heat duty gain = 19%

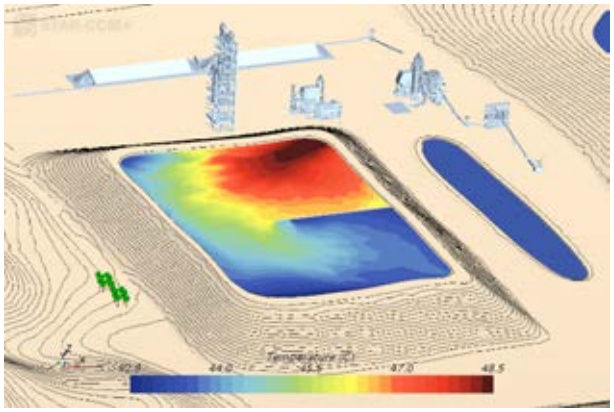


Figure 11: 1 horiz. dike, large opening, small depth

Figure 12 describes an analysis chart coming from HEEDS which allows to quickly identify trends by understanding the connections between the different design parameters. In our case it allowed to identify the following trends:

- Both horizontal and vertical dike positioning are possible
- The number of dikes may change from 1 to 7 in the best designs
- The aperture at the end of the dikes may be large or medium, depending on the number of dikes
- Depth seems to be the most influencing parameter and should be kept to a low value to improve the results.

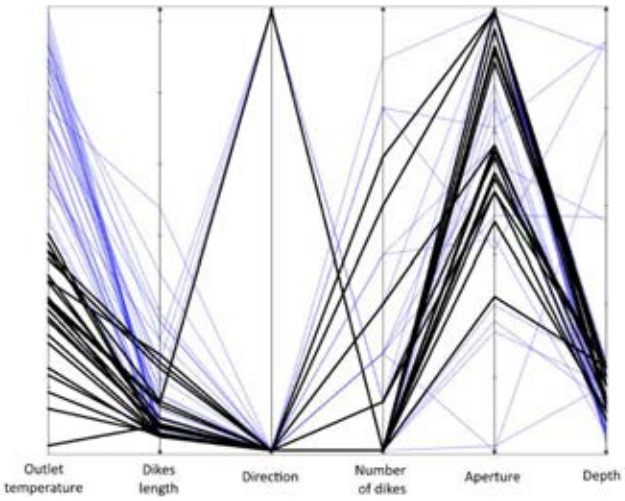


Figure 12: Connections between design parameters

CONCLUSION

Through the example of the revamping of a phosphate fertilizer plant, we have demonstrated that using CFD as a design exploration tool for large installations is no longer a pipe dream. Even without a proper 3D-CAD model to start from, different strategies to reconstruct the model into the CFD software are possible, such as using the surface wrapper tool. Although the use of this wrapping technique makes more difficult the calibration and automation of the exchanges between the CFD and Design exploration softwares, it is something achievable.

In the case we have studied, a first CFD model of the active plant configuration has been developed and the simulations that followed have allowed to quantify the heat duty provided by each of the plant cooling ponds. In order to find solutions to recover the lost duty, the multidisciplinary design exploration software HEEDS has been use to drive numerous CFD simulation runs. These calculations did not allow to establish a typical Pareto front as the defined two objectives weren't incompatible with each other. No parameters among the ones we allowed the software to explore turned out to be a real game changer by itself regarding the pond efficiency. However, a list of best designs has been determined quickly thanks to the software, allowing to increase the pond efficiency of about 20%.

While we are just starting to explore the use of design exploration software to drive our CFD simulations, this test case has shown us very promising results regarding the quantity of valuable information that can be extracted in a very short time using this approach.

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