CFD Analysis for NOx-Control in Refinery

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Abstract
In the refining business there is a large push by the industrial community to reduce emissions. Greenhouse gases as well as nitrous oxides (NO\textsubscript{x}) and sulfur dioxide (SO\textsubscript{2}) are the targeted pollutants. Governmental legislation outlined by the Environmental Protection Agency (EPA) through its MACT II guideline is a major thrust.

In refineries, downstream of process gases - cyclones, scrubbers, bag filter houses, and electrostatic precipitators are used to reduce emissions prior to gases venting to the atmosphere. The operation of this equipment is highly dependent on the humidity and temperature of the gases and so careful control must be integrated. The process of controlling the gas temperature and humidity is referred to as the gas conditioning process. Spray nozzles are an important factor in this process; spray nozzles add value by providing controlled volumes of liquid with predictable drop size and consistent spray coverage. Knowing these values remains vital for the optimization of gas conditioning processes.

In addition, the all-important placement of nozzles is often times misunderstood and therefore inaccurate. While immense care is taken to optimize placement, this often leads to failure due to the inability to predict spray performance in the application environment. This process can be facilitated by using computational fluid dynamics (CFD).

In this case study, CFD is used to identify problem areas that would have caused wetting on walls and more importantly eroded metal sections from the heavily catalyst-laden process stream. In the end, adjustments were made to original nozzle placement suggestions in order to optimize the gas conditioning process.

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Introduction

An important concern in air pollution control is the treatment of exhaust gases from power plants and industrial plants, so as to drastically limit the amount of pollutants entering the atmosphere. Electrostatic precipitators and fabric filters are commonly used to extract fly ash from coal fired boilers. These devices generally operate at temperatures greater than 390 K, with 420 K being typical. This temperature is optimal to reduce incoming gas flow temperature while maintaining adequate heat to remain above the dew point of sulfuric acid. A reduction in temperature is beneficial with respect to energy efficiency as well as required equipment size. However if the flue gas is cooled below the acid dew point, an acid mist forms which can attack the equipment downstream.

Various methods of treating flue gases are known including alkali injections, boiler preheaters and water injections. Water injections are preferable due to the relative ease of equipment retrofitting. Additional benefits to an electrostatic precipitator include: lower volumetric flow which reduces the collecting area of the precipitator, reduction in pressure drop through system and consequent energy savings, reduced temperature increases gas density thereby increasing the electric field strength for improved efficiency, reduced temperature and increased humidity results in moderate resistivity of the fly ash (1). Similarly water injections are preferable in bag houses because: lower temperature results in lower volumetric flow through the filter bags (reduction in air-to-cloth ratio results in energy savings), lower temperature reduces the gas viscosity which reduces the pressure drop, lower flow rate through filter bags increases the useful life of the filters, and increasing moisture content of the flue gas affects the porosity of the filter cake and reduces the pressure drop through the filter.

Temperature control is imperative due to the aforementioned issues. In addition, humidity must be controlled. If water injections are not fully evaporated, wall wetting and equipment damage downstream may be introduced.

Current methods rely on using spray nozzles to deliver the cooling water into the exhaust gas stream. Spray nozzles add value by providing controlled quantities of liquid and predictable drop size and spray coverage. This data is critical for effective gas conditioning. While this method has yielded some success, it has presented a series of problems due to the inability to accurately predict spray performance in the complex environment as required. Today, computational fluid dynamics (CFD) is well suited to predict flow conditions and aid in the optimization of these exhaust systems.

Today, there is no standard method in use for selecting and optimizing fluid sprays for gas conditioning applications. This paper will outline a case study in which nozzles were selected and positioned based on the critical elements of exhaust duct design and nozzle characteristics. This method consists of nozzle selection and nozzle location considerations based on known laboratory measurements of drop size, velocity and spray distribution. Furthermore, this method will also evaluate the effects of “normal” operating parameters such as exhaust gas flow rate, exhaust gas temperature, and exhaust gas velocity on exhaust uniformity and humidity.

Approach

The process of designing the gas conditioning process begins with determining the amount of liquid required for cooling and humidify the gas. In addition the optimal drop size is also determined and the drop size in this case will be a function of the dwell time.

Determining the Volume Flow Rate (VFR) requirements

The VFR requirements will greatly depend on the duct operation conditions. At a minimum the duct flow rate, duct geometry, inlet and exit temperatures must be provided. This data is used to calculate the VFR. To calculate the VFR the following assumptions are made:

- Walls are adiabatic - all heat lost by gas goes into liquid.
- Average velocity used for Mass Flow is the same as average velocity used for kinetic energy.
- Liquid volume is negligible compared to vapor volume.

Spray Cooling Requirements:

\[ H_2O (L/hr) = \frac{Q \cdot \rho \cdot S \cdot \delta T}{[(100 - T_w) + 539]} \]  

Where:
- \( Q \) = Air Flow Rate thru Duct
- \( \rho \) = Density
Determining the drop size requirements

Proper chemical interaction is dependent on liquid atomization and a controllable drop size distribution to ensure a rapid evaporation rate and eliminate a wall wetting problem causing down time (2). Wall wetting problems can be caused by atomizers that produce large drops that do not achieve full evaporation within the allowable dwell time in the duct. The process to determine the maximum allowable drop size is governed by the following equation:

\[ D(t) = \sqrt{D_0^2 - \lambda t} \]  

(2)

Where:
- \( t \) is dwell time in seconds
- \( D_0 \) is the initial diameter of the drop in microns
- \( \lambda = \frac{S_0C_p(T - T_w) \Delta T}{L \rho_{\text{gas}}} \)
- \( \Delta T \) is the Temperature Change
- \( T_w \) is the Temperature of cooling water
- \( T \) is the Gas Temperature
- \( T_{\text{wb}} \) is the Wet-Bulb Temperature of the system
- \( L \) is the Latent Heat of Vaporization of the liquid
- \( \rho_{\text{liquid}} \) is the density of the liquid.

Spray Nozzle Selection

Generally, large volume, two fluid atomizers are used in large scale industrial processes. These types of nozzles are preferred because they are able to control large and/or frequent variations in gas temperature or volume, provide consistent predictable drop size and are energy efficient.

Based on the required flow rate (VFR) and drop size values determined above, a Spraying Systems Co. FloMax® nozzle was used in this case study. The FloMax nozzle is a two-fluid, internal mix pneumatic atomizer, featuring an energy-efficient design for less air consumption. It consists of a central liquid inlet, an internal annulus ring, an internal target bolt and an air cap with eight (8) exit orifices. An array of air inlets is concentric around the central liquid inlet.

The principal of operation is as follows. Liquid impinges upon a target bolt for its initial breakup. The air stream carries the atomized liquid into the air cap. Further atomization occurs in this turbulence as well as upon exiting at each exit orifice. All testing was performed with each FloMax nozzle mounted on a single lance body. A schematic of the FM25A nozzle used in this test is show in Figure 1. Spray characterization testing was performed for several nozzles to determine optimal injection properties for the CFD model, based on the theoretical requirements.

For drop sizing, the nozzles were mounted on a 3-axis traverse. Drop size testing was performed in a single plume of the spray. Drop size measurements were executed at multiple locations, based on nozzle performance.

A two-dimensional Artium Technologies PDI-200MD instrument was used to make drop size and velocity measurements, as shown in Figure 2, the test setup is shown in Figure 3. The solid state laser systems (green 532 nm and red 660 nm) used in the PDI-200 MD are Class 3B lasers and provide about 50-60mW of power per beam. This is an intense enough laser power to help offset dense spray effects. [3, 4, 5, 6]. The test results are shown in Figure 4.
The $D_{0.5}$ and $D_{32}$ diameters were used to evaluate the drop size data. The drop size terminology [7, 8, and 9] is as follows:

$D_{0.5}$: Volume Median Diameter (also known as VMD or MVD). A means of expressing drop size in terms of the volume of liquid sprayed. The VMD is a value where 50% of the total volume (or mass) of liquid sprayed is made up of drops with diameters larger than the median value and 50% smaller than the median value. This diameter is used to compare the change in drop size on average between test conditions.

$D_{0.1}$: is a value where 10% of the total volume (or mass) of liquid sprayed is made up of drops with diameters smaller or equal to this value.

$D_{0.9}$: is a value where 90% of the total volume (or mass) of liquid sprayed is made up of drops with diameters smaller or equal to this value.

All pressures were monitored immediately upstream of the nozzle body using a 0-7 bar, class 1A pressure gauge. Liquid flow to the nozzle was delivered using a positive displacement pump. The flow rate was measured previously using a MicroMotion D6 flow meter and was correlated to nozzle pressure settings. The MicroMotion flow meter is a Coriolis Mass flow meter that measures the density of water to determine the volume flow. The meter is accurate to $\pm0.4\%$ of reading.

The Rosin-Rammler distribution function is used to convert raw measured drop data into a drop size distribution function for CFD. The Rosin-Rammler distribution function (3) is a representation of the drop population and size in a spray. The exact size for every volume fraction $F(D)$ in the spray can be calculated using the $\overline{X}$ and N parameters.

\[
F(D) = 1 - \exp\left[-\left(\frac{D}{\overline{X}}\right)^N\right]
\] (3)

Governing equations of CFD

Computational Fluid Dynamics (CFD) is the science of predicting fluid flow, heat and mass transfer, chemical reactions, and related phenomena by solving numerically the set of governing mathematical equations. For the computation the general CFD code Fluent is applied. Fluent solvers are based on the finite volume method. The fluid region is broken into a finite set of control volume (mesh). An example of this is shown below, in Figure 5.
The general conservation equations are applied. Each volume within the mesh is simultaneously solved to render the solution field. The conservation equations are shown below.

Conservation of mass:
\[
\frac{\partial}{\partial t} \alpha \rho + \nabla \cdot \alpha \rho \vec{u} = \sum \dot{m}_{in}
\]

Conservation of momentum:
\[
\frac{\partial}{\partial t} (\alpha \rho \vec{u}) + \nabla \cdot (\alpha \rho \vec{u} \otimes \vec{u}) = -\alpha \nabla P + \nabla \cdot \left( \alpha \rho \vec{F} + \sum \dot{m}_{in} \vec{u} \right)
\]

Conservation of enthalpy:
\[
\frac{\partial}{\partial t} (\alpha \rho \vec{h}) + \nabla \cdot (\alpha \rho \vec{u} \otimes \vec{h}) = -\alpha \frac{dp}{dt} + \nabla \cdot \left( \alpha \vec{w} \frac{\partial h}{\partial \vec{u}} \right) - \nabla \cdot \left( \frac{\partial h}{\partial \vec{u}} \right) + s + \sum \dot{m}_{in} \delta h
\]

Additional performance requirements:
- The nozzles must provide for a tight drop size distribution in the exhaust gas flow.
- The nozzles must feature a low spray trajectory that would insure no wall wetting.
- The injection must evaporate before the exit of the duct to avoid any damage to downstream equipment.
- The nozzles must have a large free passage to reduce clogging.

The FloMax® FM25A nozzles were selected based on laboratory testing to determine variations in spray characteristics at the required operating conditions listed in Table 1. The testing details are cited above.

**Initial Design**

**Geometry:** A detailed three-dimensional drawing of the tower duct system was drawn in CAD. The geometry was drawn based on the supplied information by the owner’s engineer. The geometry was drawn in AutoDesk® Inventor for conversion in the meshing program. The CAD representation of the initial tower duct system is shown in Figure 6, below.
The CAD drawing was imported to a 3-D volume of metric dimensions. The volume was split along the line of symmetry to decrease mesh size and improve computational convergence time. The domain was then discretized into a finite set of control volumes, known commonly as “meshing”. The mesh consists of about 1,600,000 cells. The maximum cell size for a hexagonal cell is 0.2 x 0.2 x 0.2 mm³. The standard wall function was applied with no slip conditions.

An inlet was assigned to the end of the feed pipe. Outlet conditions were assigned to each of the duct system. A total of sixteen FM25A nozzles (eight pairs of nozzles) were assigned as nozzle injections into the model. The final model with mesh and boundaries is shown in Figures 7-9, above and below.

Boundary Conditions: The segregated solver is used for the steady state solution. The realizable k-ε-model with default parameters is used for the turbulence model. Due to the height of the tower, gravity is included due to its effect on the static pressure of the flow field. The operating parameters are inserted as shown in Table 2, below.

<table>
<thead>
<tr>
<th>Pressure</th>
<th>1.1 bar</th>
</tr>
</thead>
</table>
| Reference Pressure Location
| X              | 2.74 (m) |
| Y              | 23.83 (m) |
| X              | 0 (m)    |
| Gravity (Y)    | -9.81 (m/s²) |

Table 2

The boundary conditions of the single gas flow are described shown in Table 3 below. Based on practical models, the turbulent kinetic energy is quite low, estimated at 0.1m²/s².
<table>
<thead>
<tr>
<th></th>
<th>Inlet Conditions</th>
<th>Outlet Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas Flow (kg/s)</td>
<td>54.87</td>
<td>TBD</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>922</td>
<td>616.5</td>
</tr>
<tr>
<td>Turbulence</td>
<td>Normal to Boundary</td>
<td></td>
</tr>
<tr>
<td>Turbulent Kinetic Energy (m²/s²)</td>
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<td>0.1</td>
</tr>
<tr>
<td>Turb. Dissipation Rate (m²/s³)</td>
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<td>0.1</td>
</tr>
<tr>
<td>Species/Volume Contents</td>
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<td></td>
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<tr>
<td>Water (%)</td>
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<td>18.2</td>
</tr>
<tr>
<td>Oxygen (%)</td>
<td>1.6</td>
<td>1.6</td>
</tr>
<tr>
<td>Carbon Dioxide (%)</td>
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<td>5.9</td>
</tr>
<tr>
<td>Nitrogen (%)</td>
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<td>74.3</td>
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<tr>
<td>Mass Contents</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water [1]</td>
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<td>0.121</td>
</tr>
<tr>
<td>Oxygen [1]</td>
<td>0.019</td>
<td>0.019</td>
</tr>
<tr>
<td>Carbon Dioxide [1]</td>
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<td>0.096</td>
</tr>
<tr>
<td>Nitrogen [1]</td>
<td>0.765</td>
<td>0.765</td>
</tr>
</tbody>
</table>

Table 3

For the nozzle injection modeling, the Discrete Phase Model is used. Sixteen FM25A nozzles are used at the conditions noted in Table 3. Preliminary estimations of required flow rate and drop size distribution were determined based on the desired cooling and evaporation as aforementioned. Droplet size distribution is assumed as a Rosin-Rammler distribution, based on laboratory measurements.

Modified Design

Geometry: A detailed three-dimensional drawing of the tower duct system was drawn in CAD. The geometry was drawn based on the supplied information. The geometry was drawn in AutoDesk® Inventor for conversion in the meshing program. The CAD representation of the tower duct system is shown in Figure 10, below.

The CAD drawing was imported to a 3-D volume of metric dimensions. The volume was split along the line of symmetry to decrease mesh size and improve computational convergence time. The mesh consists of about 1,800,000 cells. The maximum cell size for a hexagonal cell is 0.2 x 0.2 x 0.2 mm³. The standard wall function was applied with no slip conditions.

An inlet was assigned to the end of the feed pipe. Outlet conditions were assigned to each of the end of the duct system (Figure 11). A total of sixteen FM25A nozzles (eight pairs of nozzles) were assigned as nozzle injections into the model.

Boundary Conditions: The segregated solver is used for the steady state solution. The realizable k-ε-model with default parameters is used for the turbulence model. Unless otherwise stated inlet conditions are identical to the aforementioned case.

Results and Discussion: All modeling was performed with Fluent solvers as noted above using the aforementioned duct information. The summarized results of the models are displayed in Figures 12-25.
Figure 12. Pressure Distribution

Figure 13. Velocity Magnitude
**Figure 14.** Velocity Magnitude (m/s), $v_{\text{average}} = 42.4$ m/s @ inlet, $v_{\text{average}} = 20.3$ m/s @ outlet in negative Y-direction – Initial Design

**Figure 15.** Velocity Magnitude (m/s), $v_{\text{average}} = 40.5$ m/s @ inlet, $v_{\text{average}} = 15.9$ m/s @ outlet in negative Y-direction – Modified Design
Figure 16. Y-Velocity (m/s), section at spray injection plane, +2.5 m, +5 m, +10 m downstream and at outlet – Initial Design

Figure 17. Y-Velocity (m/s), section at spray injection plane, –1 m, +5 m, +10 m downstream and at outlet – Modified Design
Figure 18. Temperature Distribution, average 838 ºK @ inlet and 607.1 ºK @ outlet – Initial Design

Figure 19. Temperature Distribution, average 838 ºK @ inlet and 568.7 ºK @ outlet – Modified Design
Figure 20. Droplet Trajectories Coloured by Diameter (m), 25600 droplets altogether – Initial Design

Figure 21. Droplet Trajectories Coloured by Diameter (m), 25600 droplets altogether – Modified Design
Figure 22. Droplet Concentration (kg/s), 90.82% is evaporated – Initial Design

Figure 23. Droplet Concentration (kg/s), 99.55% is evaporated – Modified Design
Figure 24. Mass Fraction of H$_2$O – Initial Design

Figure 25. Mass Fraction of H$_2$O – Modified Design
The modified duct design is vastly improved from the initial planned retrofit. The initial design had substantial pressure variations throughout the duct. This is evident in Figure 14. There is a low pressure zone immediately upstream of the nozzles, which has disastrous repercussions to the flow region and ultimately the water injections. The modified design has a fairly uniform pressure in the injection area and throughout the duct geometry.

The velocity magnitude in the nozzle region varies from 100m/s to near 0m/s across the nozzle region in the initial design. This is a major issue due to the fact that all of the droplet injections need to be evaporated before they exit the duct. The theoretical estimation of evaporation is based on evenly distributed gas flow. This is due to the fact that dwell time is based on droplet size and velocity through the duct. Hence the particles in the 100m/s region of velocity are exiting the duct and are likely to cause damage to downstream equipment. The modified design has a much more uniform velocity in the nozzle / droplet injection zone. There is an approximate 20m/s variation across the nozzle zone. This allows for a more accurate theoretical assessment of evaporation, even without the nozzle injections added to the model. These trends can be seen in Figures 16-17.

Further assessment of the velocity profiles are shown in Figures 14-15. The vector velocity in the initial design shows several regions of reverse flow. Again the flow in the nozzle zone is not ideal. Reverse flow is shown in half of the nozzle region. Once more this is detrimental to the designed quench system and often times leads to the impingement of droplets on internal walls. It also causes liquid droplets to flow upstream and impact the lances. If there is gaseous state acids that combine with the water, acidic corrosion issues can arise. This also is likely to inhibit adequate evaporation of injected droplets. The asymmetric flow may also interfere with the intended path of the droplets and may result in wall wetting. There is a second region of reversed flow at the outlet of the duct. This is a minor problem assuming that the droplets are evaporated at the exit of the duct.

The velocity profiles of the modified design are shown in Figure 15. There is some reversed flow within the turning vanes prior to the nozzle zone. However at the point of droplet injection the gas flow is fairly uniform and moving in a single direction. This is a key improvement to the quench design. Again there is a minor issue with reversed flow at the exit of the duct.

Temperature distribution throughout the duct was examined. This temperature is critical to the gas conditioning process. The initial design exhibited hotspots in the length of the duct and uneven cooling of the gas exiting the duct. The design modification improved the temperature deviation from the target temperature as well as the uniformity with respect to temperature of flue gas at the exit of the duct. These trends are evident from examination of Figures 18-19.

Droplet trajectories were tracked for each design iteration. The results of these models can be seen in Figures 20-21. These Figures are very telling with regards to quench effectiveness. The initial design indicates reversed motion of liquid droplets. This phenomenon will cause wall wetting in the duct. It is also quite likely that these droplets will coalesce in the nozzle zone creating large droplets that will not have adequate dwell time to evaporate prior to the exit of the duct. Overtime, the recycling motion of the droplets also has the potential to build up on the nozzle face adversely effecting spray performance.

This phenomenon follows through to the evaporation and water content of the flue gas as it approached the exit of the duct. The evaporation and water content trends are displayed in Figures 22-25. Again the modified duct design demonstrates improved characteristics, with an 8% improvement in evaporation of injected droplets.

Conclusions

In the reduction of air pollution emissions, quench systems are often used to reduce temperature in the removal of fly ash from coal-fired boilers. Quench systems require a highly controlled, predictable and repeatable spray to function effectively. Due to the expense and effort required to add a spray system, a computational fluid dynamics (CFD) study for a quench vessel was examined to determine feasibility prior to purchase or installation. The model includes a detailed three dimensional representation of the geometry near the injection area and downstream.

A method for optimizing spray nozzle choices and placement used in gas conditioning applications was presented in this work. The approach consists of optimizing the gas flow and determining adequate quench spray and evaluating the effects of “normal” operating parameters such as fluid flow rate, atomization pressure, and gun location on flow uniformity, evaporation, and gas temperature. All tests conducted in this study were performed using water.
Theoretical estimation of the required amount of liquid required for cooling and humidify the gas was determined. In addition the optimal drop size was estimated relative to droplet dwell time. Various nozzles were selected and tested to determine actual spray characteristics at various operating conditions. The FM25A nozzle was experimentally determined to be the optimal nozzle for this application.

A baseline study of the flue gas flow through the planned retrofit ductwork was done with CFD. The results of this initial design were potentially disastrous. From Figures 12-25, it is evident that there is extensive wall wetting occurring upstream of the water injections. This is due to reversed flow in the duct. Flow through the planned ductwork was shown to have several areas of non-uniform and turbulent flow. This asymmetric flow did not allow for complete evaporation and also resulted in ‘hot spots’ and over cooled areas within the duct. These problems have potential to cause wall wetting and potential for acidic buildup. Hence this design could have wreaked havoc on the duct and downstream equipment.

Through an iterative optimization process a substantial improvement in the duct design was revealed. At the base line condition, the turbulence and gas flow variation was extremely high with detrimental effects to temperature distribution (gas cooling) and droplet evaporation. Through subsequent iterations the gas flow uniformity was vastly improved (Figures 12-17). Velocity across the nozzle region improved from a ±75m/s velocity range to a ±20m/s range. In addition the reversing flow in the nozzle range was eliminated with modified duct geometry.

The improvements to the flow uniformity carried through to improvements in temperature distribution and droplet evaporation. The modified duct design improved the average temperature exiting the duct as well as the uniformity of the temperature exiting the duct. The final duct design indicated an average exit temperature of 568.7 °K and a 99.5% evaporation of the quench water. There were no indications of potential for wall wetting within this design. This result was deemed to be within an acceptable range for this application.

More work may be desired in order to improve the duct design and improve the gas condition effect in this application. Some minor adjustments to nozzle flow rate and drop size may allow for additional cooling as desired.

REFERENCES
1. Aa, Peter, "Reviving an Electrostatic Precipitator", hamon-researchcottrell.com, November, 1991

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