Optimization of SO2 Scrubber using CFD Modeling

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Abstract

The reduction of environmental contaminants that contribute to smog and soot is a worldwide goal that has seen an increased focus in recent years. In the United States, for example, it is estimated that by 2014 new rules will lead to a 71% reduction of sulfur dioxide emissions and 52% of nitrogen oxide emissions as compared to 2005 level. Thus, medium-sized plants (100-500MW) that currently do not have flue gas desulfurization (FGD) units or selective catalytic reduction systems (SCRs) will be required to adapt. Similar emission reduction efforts are expected to be adopted globally, albeit at different levels. Wet-scrubber FGD is characterized as one of the most effective SO_2 removal techniques with low operating costs. However capital cost for implementation is considered high. Hence an effective optimization procedure is required to reduce these capital costs of conversion.

Power plants commonly use a lime slurry spray reaction to reduce SO_2 emissions. Control of the droplets throughout the tower geometry is essential to ensuring maximum reduction while minimizing scale. The liquid slurry is known to have density, surface tension and viscosity values that deviate from standard water spray characteristics, which complicates process optimization. In order to improve the scrubber, nozzle characteristics and placement must be optimized to reduce the cost of the system implementation and mitigate risks of inadequate pollution reduction. A series of large flow rate, hydraulic, hollow cone sprays were investigated for this study.

A Computational Fluid Dynamics (CFD) model was used to examine potential scrubber designs for optimization of the system. Nozzle parameters were modeled to allow particle tracking through the system. An ANSYS Fluent Lagrangian particle tracking method was used with heat and mass transfer. The alkaline sorbent material and SO_2 reaction is modeled to determine uniformity and efficacy of the system. Volumetric chemistry mechanisms were used to simulate the reaction. These results demonstrate the expected liquid-gas interaction relative to the system efficiency. Drop size, liquid rheology, and spray array layout were examined to achieve SO_2 removal above 90%. Wall impingement and flow pattern results were evaluated due to their impact in minimizing equipment plugging and corrosion required as for long-term scrubber utilization.

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Introduction

The reduction of environmental contaminants that contribute to smog and soot is a worldwide goal. As restrictions on emissions increase around the world, there is a global need for upgrades or additions to pollution control systems. Based on current regulation projections, medium-sized plants (100-500MW) that currently do not have flue gas desulfurization (FGD) units or selective catalytic reduction systems (SCRs) will be required to adapt in a short timeframe. Wet-scrubber FGD is characterized as one of the most effective SO_2 removal techniques with low operating costs. However capital cost for implementation is considered high. Hence an effective optimization procedure is required to reduce these capital costs of conversion.

Process improvement and optimization is a constantly ongoing effort. Power plants commonly use a lime slurry spray reaction to reduce SO_2 emissions. Droplet size introduced into the tower is essential to ensuring maximum reduction while minimizing scale. The liquid slurry is known to have density, surface tension and viscosity values that deviate from standard water spray characteristics, which complicates process optimization. The improvements made in nozzle design and liquid atomization, in recent years, have provided the possibility of process optimization like never before. In order to improve the scrubber, nozzle characteristics and placement must be optimized to reduce the cost of the system implementation and mitigate risks of inadequate pollution reduction. In situ analysis would provide the best assessment of a spray's characteristics in the tower, however often this is cost prohibitive or not physically possible. In lieu of inline optimization, computational fluid dynamics (CFD) projects for this type of application have become very useful. With CFD, gas conditioning process engineers are able to assess the spray quality within the actual spray process region.

Spraying Systems Co. has the unique combination of testing and modeling expertise that allowed for a rigorous validation of spray modeling techniques often used to simulate un-testable situations. This body of work relates to the analysis of various injectors to examine their efficacy in SO_2 reduction, using a lime slurry injection. The nozzles were characterized using Phase Doppler Interferometry (PDI) to determine drop size distribution and velocity at various operating conditions. This data is used to provide accurate input to model the FGD process.

Equipment and Methods

### Test Setup and Data Acquisition

For drop sizing, the nozzle was mounted on a fixed platform in a vertical downward orientation. The data was acquired at 600mm downstream of the nozzle exit orifice. Drop size and velocity information was collected at various operating conditions. Multiple points throughout the spray plume were measured with a mass and area weighted average reported for comparison purposes.

A two-dimensional Artium Technologies PDI-200MD [9, 10] system was used to acquire drop size and velocity measurements. The solid state laser systems (green 532 nm and red 660 nm) used in the PDI-200MD are Class 3B lasers and provide 50-60mWatts of power per beam. The lasers were operated at an adequate power setting to overcome interference due to spray density.

The transmitter and receiver were mounted on a rail assembly with rotary plates; a 40° forward scatter collection angle was used. For this particular test, the choice of lenses was 1000mm for the transmitter and 1000mm for the receiver unit. This resulted in an ideal size range of about 4.0µm – 1638µm diameter drops. The optical setup was used to ensure acquisition of the full range of drop sizes, while maintaining good measurement resolution. The particular range used for these tests was determined by a preliminary test-run where the $D_{V0.5}$ and the overall droplet distribution were examined. For each test point, a total of 10,000 samples were acquired. The experimental setup can be seen in Figures 1and 2.
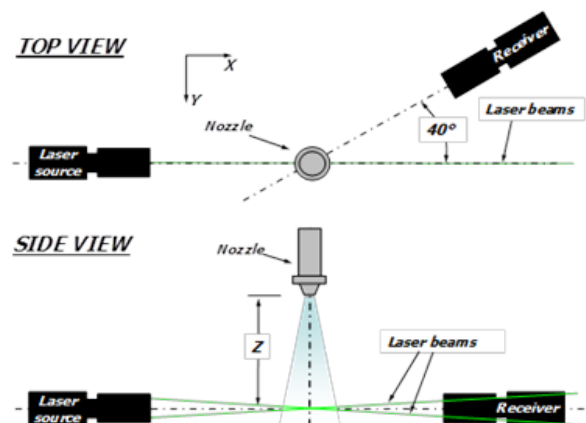
Figure 1. Illustration of PDI layout for drop size and velocity data acquisition.
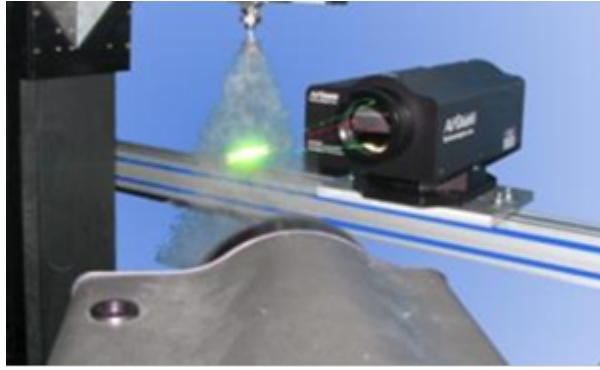
Figure 2. Illustration of PDI during experiment.

The $D_{V0.1}$, $D_{V0.5}$, D_{32}, and $D_{V0.9}$ diameters were used to evaluate the drop size data. This drop size terminology is as follows:

$D_{V0.1}$: 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_{32}: Sauter Mean Diameter (also known as SMD) is a means of expressing the fineness of a spray in terms of the surface area produced by the spray. SMD is the diameter of a drop having the same volume to surface area ratio as the total volume of all the drops to the total surface area of all the drops.

$D_{V0.5}$: 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 equal to or smaller than the median value. This diameter is used to compare the change in average drop size between test conditions.

$D_{V0.9}$: 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.

By analyzing drop size based on these standardized drop statistics it is possible to objectively characterize the quality and effectiveness of this atomizing nozzle for the prescribed application.

Test Fluids and Monitoring Equipment

All testing was conducted using water and solution to simulate the fluid properties of lime slurry. Flow to the system was supplied using a high volume pump. The liquid flow rate to the injector was monitored with a MicroMotion flow meter and controlled with a bleed-off valve. The MicroMotion flow meter is a Coriolis Mass flow meter which measures the density of the fluid to determine the volume flow. The meter is accurate to 0.4% of reading. Liquid pressures were monitored upstream of the injector with a 0-1.03MPa, class 3A pressure gauge.

Injectors

Total five types of injectors were evaluated to determine the effectiveness for this application. The injectors were full cone, narrow style injectors, of the Spraying Systems Co. FullJet® style. Two injectors were selected based on a target flow rate of 37.85 lpm flow, another three injectors were selected for target of 30.28 lpm. Multiple capacity sizes and configurations were used to achieve this design requirement.

Numerical Simulations

CFD Background

Computational Fluid Dynamics (CFD) is a numerical method used to numerically solve fluid flow problems. Today's CFD performs use extremely large number of calculations to simulate the behavior of fluids in complex environments and geometries. Within the computational region, CFD solves the Navier-Stokes equations to obtain velocity, pressure, temperature and necessary chemical reactions for removal of SO_2. Recently CFD became a popular design and optimization tool with the help of commercially available software and advancing computer technology. The commercially available CFD package ANSYS FLUENT (version 14) was used for the simulation

Simulation Description

Figure 4, shows a pilot wet absorber that has a capacity of 6 million Btu/hr. This geometry was used for the model of the high velocity absorber [1]. The absorber has a gas flow capability of 4000 acfm, with SO_2 concentrations up to 6000 ppmdv. The gas flow comes in from the inlet and continues through the absorber turn to the outlet. Liquid slurry enters from the injector(s) and moves out from the system at quenching zone. The importance of the pollutant removal process is determined through the observation of the gas liquid interactions at the tray, improved by optimization of the injector system.

Air and reacting gases inside the horizontal scrubber were set as primary phase flow (Eulerian approach). The primary phase used coupled models (momentum, turbulence, energy, species mixing and reaction) which required boundary conditions (BC's). This simulation consisted of inlet BC and outlet BC, set as "mass flow rate inlet" and "constant pressure outlet" respectively. The calcium carbonate injection was set as secondary phase (Lagrangian approach) where its inlet BC's are based on spray injection parameters as determined empirically. The Lagrangian particles were set using "wet combustion" models. The Lagrangian particles were tracked using Discrete Phase Model (DPM). During computation, heat and mass transfer was coupled be-

tween primary and secondary phases. CFD Multiple Surface Reaction Model set-up reaction kinetic parameters and factors are extracted and calculated through experimental results from Wang [6] and probabilities method from Krebs [7].

To generate the computation domain (mesh) for the scrubber shown in Figure 4, ANSYS workbench mesher (version 14) was utilized. The mesh consisted of (single injector configuration) 44003 polyhedral cells and 217150 faces; (two injector configuration) 53897 polyhedral cells and 273068 faces; (three injector configuration) 64391 polyhedral cells and 332411 faces, minimum cell size is 1e-5m. Due to its size and modeling complexity, the simulation required significant computer power and processing time. The walls had a common (standard) setup, with no slip, adiabatic (insulated) and reflect for the combusting particles.
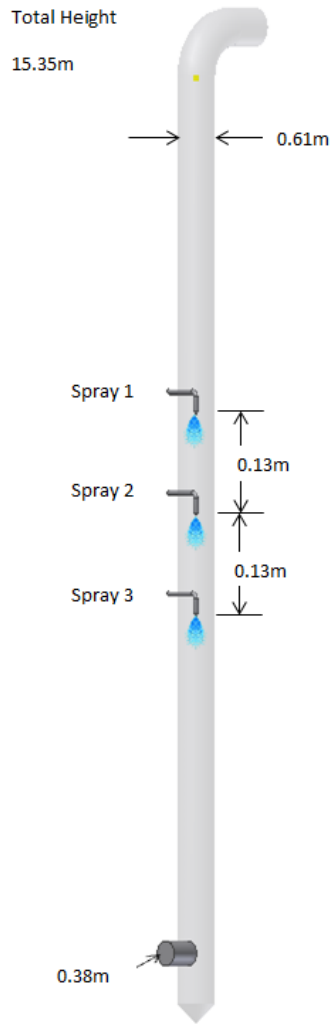

Figure 4. CFD Scrubber Geometry

Wet Combustion Particle Surface Reaction

Computational fluid dynamic (CFD) simulation is mainly using ANSYS Fluent Wet combustion particle surface reaction chemistry models, which have been developed and parametric tested during simulations. ANSYS Fluent can model the mixing and transport of chemical species by solving conservation equation describing convection, diffusion, and reaction sources by its multiple surface reaction models [4].

Reaction occurred in the bulk phase is dealt with volumetric reaction, and particle surface reaction. For gas-phase reactions, the reaction rate is defined on a volumetric basis and the rate of creation and destruction of chemical species. Particle surface reaction is used to model surface combustion on a discrete-phase particle. In the discrete phase model, modeling multiple particle surface reactions makes the surface species as a "particle surface species".

The initial relationship for calculating particle burning rates were presented and discussed by Smith [5]. The particle reaction rate, $\mathcal{R}$ (kg/m2·s), can be expressed as

$$\mathcal{R} = D_0 (C_g - C_s) = R_c (C_s)^N \tag{1}$$

In above equation, the concentration at the particle surface, C_s, is unknown and eliminated as follows:

$$\mathcal{R} = R_c [C_g - \mathcal{R} / D_0]^N \tag{2}$$

This equation has to be solved by an iterative procedure in Fluent, with the exception of the cases when N=1 or N=0, which can be written as

$$\mathcal{R} = \frac{C_g R_c D_0}{D_0 + R_c} \tag{3}$$

In the case of N=0, if there is a finite concentration of reactant at the particle surface, the solid depletion rate is equal to the chemical reaction rate. If there is no reactant at the surface, the solid depletion rate changes abruptly to the diffusion-controlled rate. ANSYS Fluent will always use the chemical reaction rate for stability reasons.

Based on the above explanation, ANSYS Fluent uses the following equation to describe the rate of reaction r of a particle surface species j with the gas phase species n. The rate is given as

$$\overline{\mathcal{R}}_{j,r} = A_p \eta_r Y_j \mathcal{R}_{j,r} \tag{4}$$

$$\mathcal{R}_{j,r} = \mathcal{R}_{kin,r} \left(p_n - \frac{\mathcal{R}_{j,r}}{D_{0,r}} \right)^N \tag{5}$$

The effectiveness factor is related to the surface area, which can be used in each reaction in the case of multiple reactions. $D_{0,r}$ is given as

$$D_{0,r} = C_{1,r} \frac{\left[\left(T_p + T_\infty \right)/2 \right]^{0.75}}{d_p} \quad (6)$$

The kinetic rate of reaction r is defined as

$$\mathcal{R}_{kin,r} = A_r T_p^{\beta_r} e^{-\left(E_r/RT_p \right)} \quad (7)$$

The rate of the particle surface species depletion for reaction order $N_r = 1$ is given by

$$\overline{\mathcal{R}}_{j,r} = A_p \eta_r Y_j p_n \frac{\mathcal{R}_{kin,r} D_{0,r}}{D_{0,r} + \mathcal{R}_{kin,r}} \quad (8)$$

For reaction order $N_r = 0$,

$$\overline{\mathcal{R}}_{j,r} = A_p \eta_r Y_j \mathcal{R}_{kin,r} \quad (9)$$

The surface reaction consumes the oxidant species in the gas phase, also consumes or produces energy, in an amount determined by the heat of reaction. The particle heat balance during surface reaction is

$$m_p c_p \frac{dT_p}{dt} = h A_p \left(T_\infty - T_p \right) - f_h \frac{dm_p}{dt} H_{reac} + A_p \varepsilon_p \sigma \left(\theta_R^4 - T_p^4 \right) \quad (10)$$

It includes the diffusion and convection control of the vaporization model.

Results (Experimental and Numerical)

Experimental Results

The results of the PDI measurements provide a representative characterization of the atomizer effectiveness at the 600mm downstream investigation location. As outlined and described in the above sections, the results from testing are provided in Table 1 and 2. The Volumetric Mean Diameter ($D_{V0.5}$) as well as other representative diameter statistics based on the volume flow is presented. These results allow the evaluation, qualitatively, of the dependence of drop size on the liquid flow rate and pressure.

There are notable trends that persist throughout the data. With an increase in liquid feed pressure, there is a decrease in median drop size and an increase in mean drop velocity.

Preliminary Study CFD Results

One to three injectors were evaluated in series to determine optimal design parameters. All simulations were performed with a consistent total mass flow rate of 37.9 lpm. The effect of the injector is evaluated to allow for a design with minimal waste and wall contact, to improve efficacy and decrease the required maintenance of the system. The results indicated the SO2 mass fraction in each case and SO2 removal for each case. Velocity magnitude and vertical velocity profile, discrete phase concentration and particle tracking is

Nozzle ID	units	1HH-SS 3070	1/2GG-SS 3030	1/2GG-SS 3030	1/2GG-SS 3030
Pressure (dP)	Pa	565370	765318	275790	489528
$D_{V0.5}$	micron	539	443	635	530
Distribution Parameter		2.5	2.5	2.5	2.5
Injected Flow	lpm	37.9	18.9	11.4	15.1
No. of Spray Levels		1	2	3	3

Table 1. Drop Size and Velocity Results of Empirical Investigation in Preliminary Study.

Nozzle ID	units	3/8G-9.5 FullJet	3/8GANV-13 FullJet	special 3/4GG-3 FullJet
Pressure (dP)	Pa	655002	655002	565370
DV0.5	micron	526	464	510
Distribution Parameter		2.39	3.36	2.55
Injected Flow	lpm	10.22	15.14	30.28
No. of Spray Levels		3	2	1

Table 2. Drop Size and Velocity Results of Empirical Investigation in Follow-up Study.

shown to better understand the flow behavior and pattern in the scrubber. Case comparison is shown in Table 3.

All cases achieve full SO2 reduction as designed. Three-nozzle scrubber has the best SO2 removal capability, based on calcium carbonate consumption. Similarly, the two-nozzle scrubber shows a greater removal than one-nozzle scrubber with less calcium carbonate consumption at the same supply quantity. This result indicates a trend relating smaller drop sizes to greater efficacy of SO2 removal. Due to the relationship of drop size volume to surface area, with equivalent volume introduced into the system, it is possible to significantly increase surface area and associated surface reaction rate in the tower. Moreover, increasing spray zone flow distribution will lead to higher efficiency. The velocity behavior exhibits less oscillation and recirculation than the in the three-nozzle scrubber at the same high inlet velocity. However, it causes adverse results with respect to wall wetting. It should be noted that there is an especially high concentration area formed around spray zone, which is greater than expected. Wall impingement may cause equipment erosion when injection fluid has corrosive property.

In the three nozzle case, at 11.4 and 15.1 lpm supply quantity, more supply does not show better SO_2 reduction with smaller drop size. This may be due to the fact that the 11.4 lpm supply case has already achieved 18.89% of slurry consumption. The marginal reduction in drop size my not have significant effect on slurry consumption at this level. Also, the 15.1 lpm supply case has a total injection quantity of 45.4 lpm, when accounting for all injectors. This flow could be too much for the scrubber at this input condition, which might lead to less efficiency by slurry accumulation. These results may need further research to determine cause and effect of this result.

The results presented herein, represent a preliminary work for SO_2 removal based on different nozzle designs. From the net species mass flow table, it clearly shows the slurry consumption is below 50% for all the cases to remove targeted pollutants. The slurry injection quantity, effective usage research will be one of the further major subjects to improve scrubber efficiency.

Considering the slurry flow behavior from the simulation result, high velocity inlet helped with the SO_2

fully removal, while it also caused concerns relating to undesirable wall interactions. Therefore, a range of different velocity inlet tests on the influence of nozzle selections, wall wetting and pollutant removal efficiency could make further improvements on this research.

Furthermore, as discovering the nozzle efficiency, several tests could be made to get relationship between nozzle supply quantity and nozzle provided droplet size for higher removal capability achievement.

Follow-up Study CFD Results

Based on previous result, a series of new designs have been investigated to study system optimization. One to three injectors were evaluated in series to determine optimal design parameters. All simulations were performed with a consistent total mass flow rate of 30.28 lpm. The effect of the injector was evaluated to allow for a design with minimal waste and wall contact, to improve efficacy and decrease the required maintenance of the system. The results indicate the SO_2 mass fraction in each case and SO_2 removal for each case. Velocity magnitude and vertical velocity profile, discrete phase concentration and particle tracking is shown to better understand the flow behavior and pattern in the scrubber. Case comparison is shown in Table 4. And simulation results are presented in Figure 5 to 7.

From the DPM concentration contours, it can be seen that wall impingement is heavier when there are multiple nozzles applied in the cases corresponding with high speed flow in the scrubber, due to the wider droplet spread area. However optimal nozzle location could reduce wall impingement even for multiple nozzle application as shown in three nozzle cases.

Multiple-nozzle applications lead to much quicker pollutant removal than single-nozzle set-up when removal process can be achieved.

Optimal nozzle locations will affect the removal efficiency and wall impingement benefiting from uniformly distributed droplet distribution. As in the dual-nozzle cases, the big interval creates maximum wall wetting and causes slurry accumulation, which the situation is weakened in triple-nozzle cases. Poor nozzle locations decrease the pollutant removal efficiency, and hence should be selected with care.

Case Name	net species mass flow	O2	SO2	CO2	CaCO$_3$ Slurry Consumption
1 Nozzle Injection	kg/s	0.01854	0.06198	-0.05213	26.97%
2 Nozzle Injection	kg/s	0.01592	0.06203	-0.04799	19.33%
3 Nozzle Injection	kg/s	0.01643	0.06187	-0.05345	18.89%

Table 3. SO$_2$ Scrubber CFD Simulation Species Data in Preliminary Study.

The results follow the trends observed with previous study.

Low velocity inlet cases show better SO_2 removal capability than high velocity inlet. Meanwhile, test cases give out an opposite slurry consumption trend to SO_2 removal. Low velocity inlet cases use less slurry than high velocity inlet cases. However, pure calcium carbonate (lime component) usage is not following this rule in the comparison, which almost has the same motion as SO_2 removal.
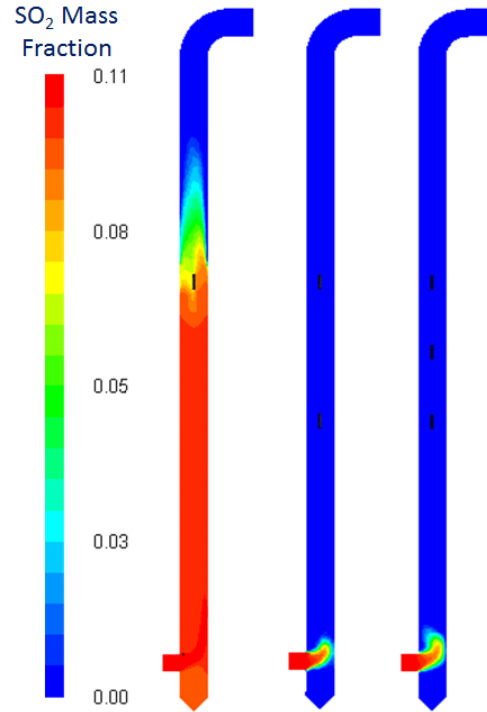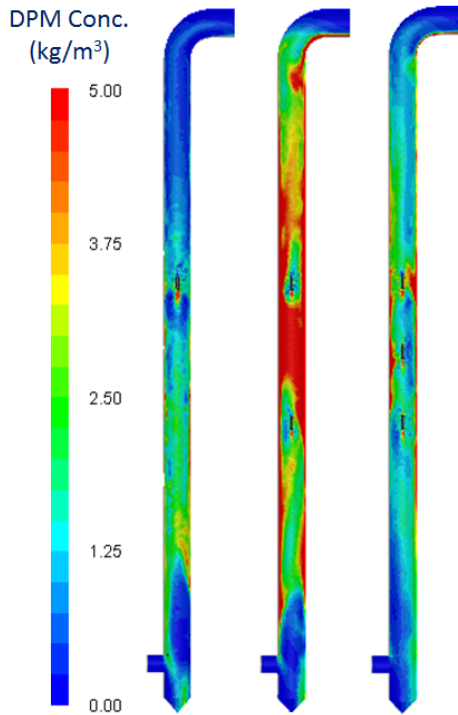
Figure 5. Pollutant Removal Situations for 1, 2 and 3-Nozzle Applications @ Velocity of 18 ft/s.

From above it indicates slurry consumption also includes the consumption of water component in slurry consumed by evaporation process. Since wet scrubbing process applies lime slurry in spray towers to eliminate SO_2, this process is significantly influenced by water. Dilute lime slurry could cause the result varies because of water evaporation and diffusion process. This study is using a type of dilute slurry as spray injection agent, which is different than previous simulation.

Nozzles chosen in this study are based on the same target capacity (which still meets the same total carry amount for each nozzle quantity, but less than previous), coming from different type of the same product catalog (FullJet®) and having different injection properties. The Sauter mean drop size diameter (SMD) produced by these nozzles is adjusted to be the same. Under this condition, the total surface area of the droplets will be the same, which helps to see the relationship of spray distribution and removal capability:
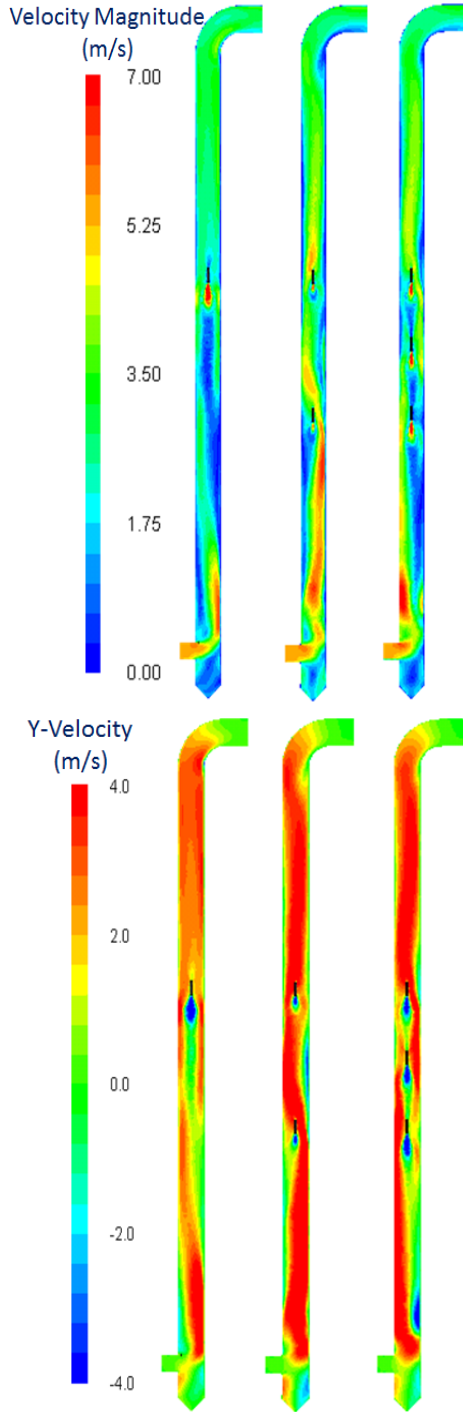
Figure 6. Flow Profiles for 1, 2 and 3- Nozzle Applications @ Velocity of 18 ft/s.

For the low inlet velocity input, cases with one nozzle show a slightly better removal rate than multiple nozzles. The reason for this situation may come from the nozzle characterization combined with less water diffusion advantages in low velocity for single nozzle cases since it is shown lime consumption is actually bigger than others. From the 16ft/s and 18ft/s velocity inlet cases, three nozzles removal rate is absolutely better than two nozzles and close to one nozzle. Also its pure lime consumption and total slurry consumption is lower than the single nozzle layout.

At the highest velocity inlet (20ft/s), SO_2 removal rate is 3 nozzles > 2 nozzles > 1 nozzle. Following this order, corresponding pure lime consumption is greater, and total slurry consumption is less. Therefore, under high inlet velocity conditions, water evaporation and diffusion will slow down which helps the pollutant removal reaction process. However, due to less contact time, the removal capacity is much less than other velocities cases.
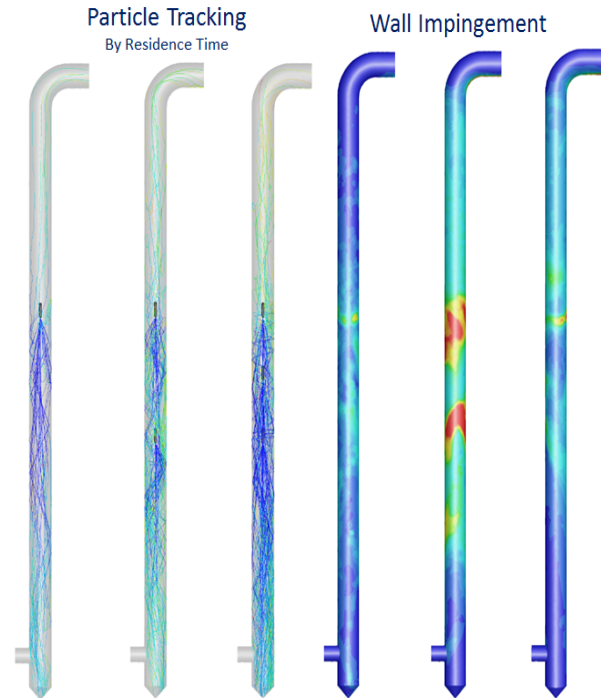
Figure 7. Particle and Wall Wetting Conditions for 1, 2 and 3- Nozzle Applications @ Velocity of 18 ft/s.

Conclusion

High speed inlet velocity helps forward reaction. One reason is due to weakened influence by the speed of water evaporation and diffusion, resulting from water component in the slurry. While high speed also causes less residence time with pollutant gas, there is also a reduction in the removal capability. Therefore, choosing a proper high speed velocity is important in SO_2 wet scrubbing process.

Also, multiple nozzle locations helps removal process, as the slurry droplets have a more uniform and wide distribution. However, this also allows for water species in dilute slurry attain similar rapid evaporation inhibiting against the SO_2 removal reaction. In this study, the single nozzle at 16ft/s and 18ft/s inlet flow presents an outstanding removal performance, which

may result from the non-wide spread water species while it also consumed more lime than others. It is inferred the nozzle characterization like high injection speed provided by nozzle helps with slowing down effect of water component. Nozzle injection location is also an important factor of removal capability for avoiding accumulation and wall wetting.

The balance of high speed inlet gas flow and nozzle selection, locations will optimize removal process, increase the pollutant removal efficiency, and save expenditures on slurry consumption. Since water species has significant influence on wet scrubbing technology calcium carbonate absorbing sulfur dioxide, nozzle performance tests are required before it is applied to the scrubber.

Through the optimal result, more application designs can be made based on nozzle properties to develop spray behavior and decrease erosion on the walls with the requirement of standard removal or even better. Future studies are planned to further develop computational models and increase understanding of FGD scrubber systems.

Acknowledgements

Nomenclature

$u_{\circ}$	velocity in the direction of (m/s)
A	radius of (m)
B	position of
C	further nomenclature continues down the page inside the text box
D_0	bulk diffusion coefficient (m/s)
C_g	mean reacting gas species concentration in the bulk (kg/m^3)
C_s	mean reacting gas species concentration at the particle surface (kg/m^3)
R_c	chemical reaction rate coefficient (units vary)
A_p	particle surface area (m^2)
Y_j	mass fraction of surface species j in the particle
η_r	effectiveness factor (dimensionless)
$\mathcal{R}_{j,\,r}$	rate of particle surface species reaction per unit area (kg/m2·s)
$\overline{\mathcal{R}}_{j,r}$	rate of particle surface species depletion (kg/s)
p_n	bulk partial pressure of the gas phase species (Pa)
$D_{0,r}$	diffusion rate coefficient for reaction r
$\mathcal{R}_{kin,\,r}$	kinetic rate of reaction r (units vary)
N_r	apparent order of reaction r

Greek symbols

γ	stoichiometric coefficient
δ	boundary layer thicknesses(m)

Subscripts

r	radial coordinate

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