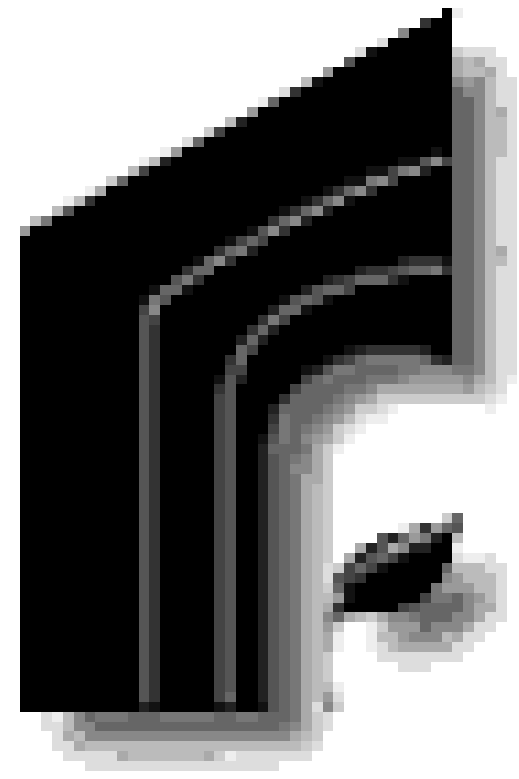
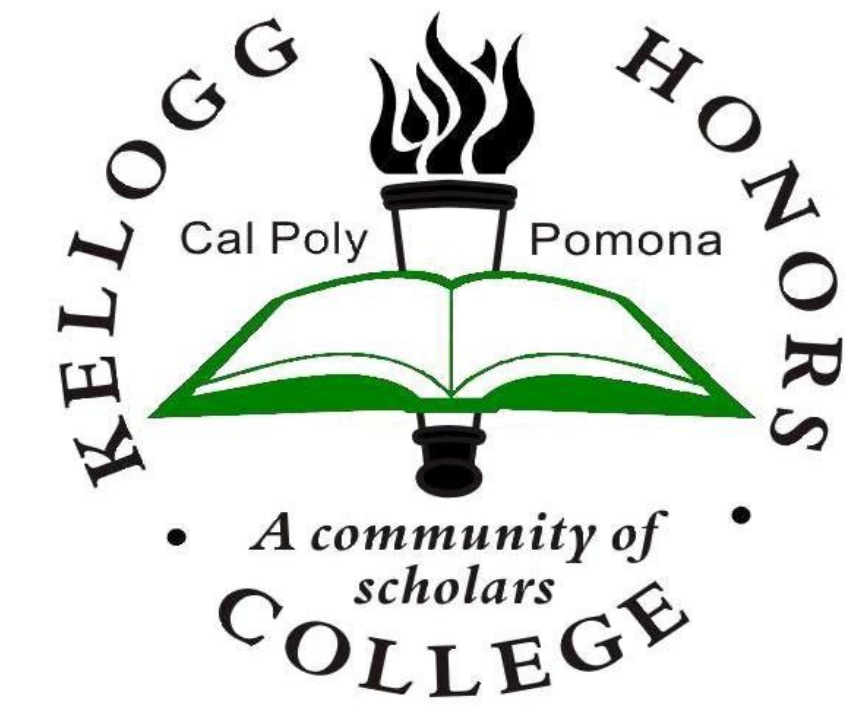


Computational Modeling of a Flue Gas Desulfurization Reactor



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Kellogg Honors College Capstone Project



Background:

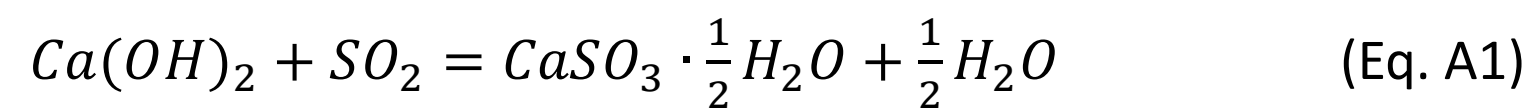
Overall Process:

A Flue Gas Desulfurization (FGD) Reactor is a typical unit operation used to absorb and remove sulfur dioxide from a given process stream using lime slurry as a sorbent in order to meet strict SO₂ emission levels. The type of FGD reactor that is of importance in this study is a Backmixed Spray Dryer as shown in **Figure 1** given the high degree of mixing that is common amongst spray dryers leading the slurry droplet to be exposed to a constant environment of SO₂ laden flue gas. The absorption process begins when the flue gas enters the spray dryer co-currently alongside the lime slurry droplet containing Ca(OH)₂ particles. The residence time of the flue gas is typically 10 seconds. Three mass transfer mechanisms occur within the spray dryer: the water evaporation of the droplet, absorption of SO₂ by the slurry droplet, and the dissolution of the lime sorbent. Make-up water is added to the prepared slurry in order to control the inlet temperature of the spray dryer and the approach to saturation temperature. The drying of the slurry droplet is independent of the SO₂ absorption process while the SO₂ absorption is dependent on the drying process as the presence of moisture increases the reaction rate of the ionic reaction between the two species.

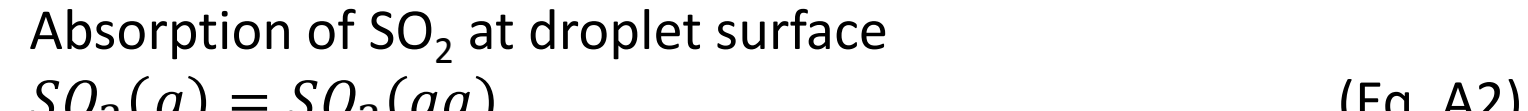
Reaction Chemistry:

The absorption of SO₂ by a slurry droplet can be broken down into three diffusion steps, the first being gas phase diffusion of SO₂ from the bulk gas phase to the droplet surface as shown in **Figure 2**. Liquid phase diffusion occurs where SO₂ is transported from the liquid-gas interface to the interior of the droplet. The calcium hydroxide on the other hand, dissolves from the solid phase and past the liquid film surrounding the particle to the bulk liquid region on the RHS of the concentration profile. If the ionic reaction between the sulfur dioxide and the calcium hydroxide particles are fast, as they are in the wet particle phase, both species will then migrate to a reaction zone shown in the middle of **Figure 2**.

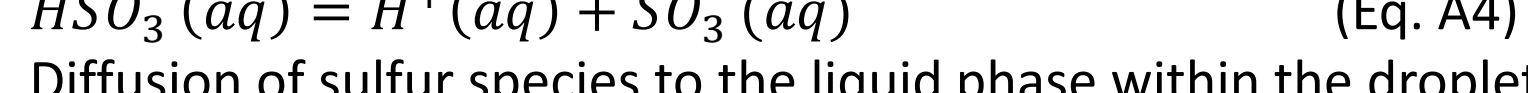
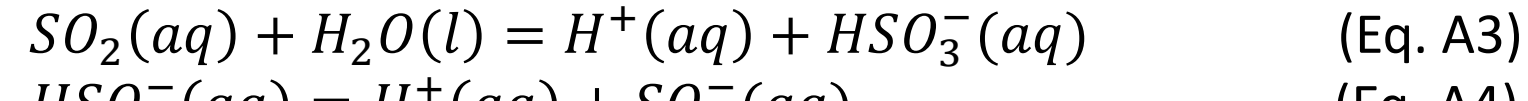
Overall Reaction:



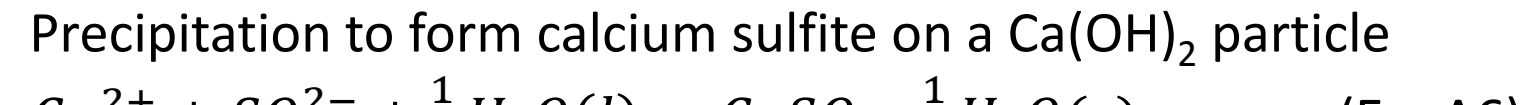
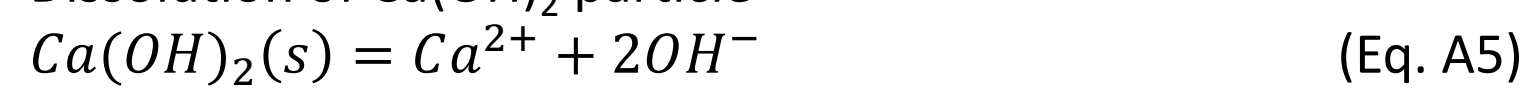
Diffusion of SO₂ from the bulk gas to the droplet surface



Interception of dry sorbent particles to the droplet



Diffusion of sulfur species to the liquid phase within the droplet



Precipitation to form calcium sulfite on a Ca(OH)₂ particle

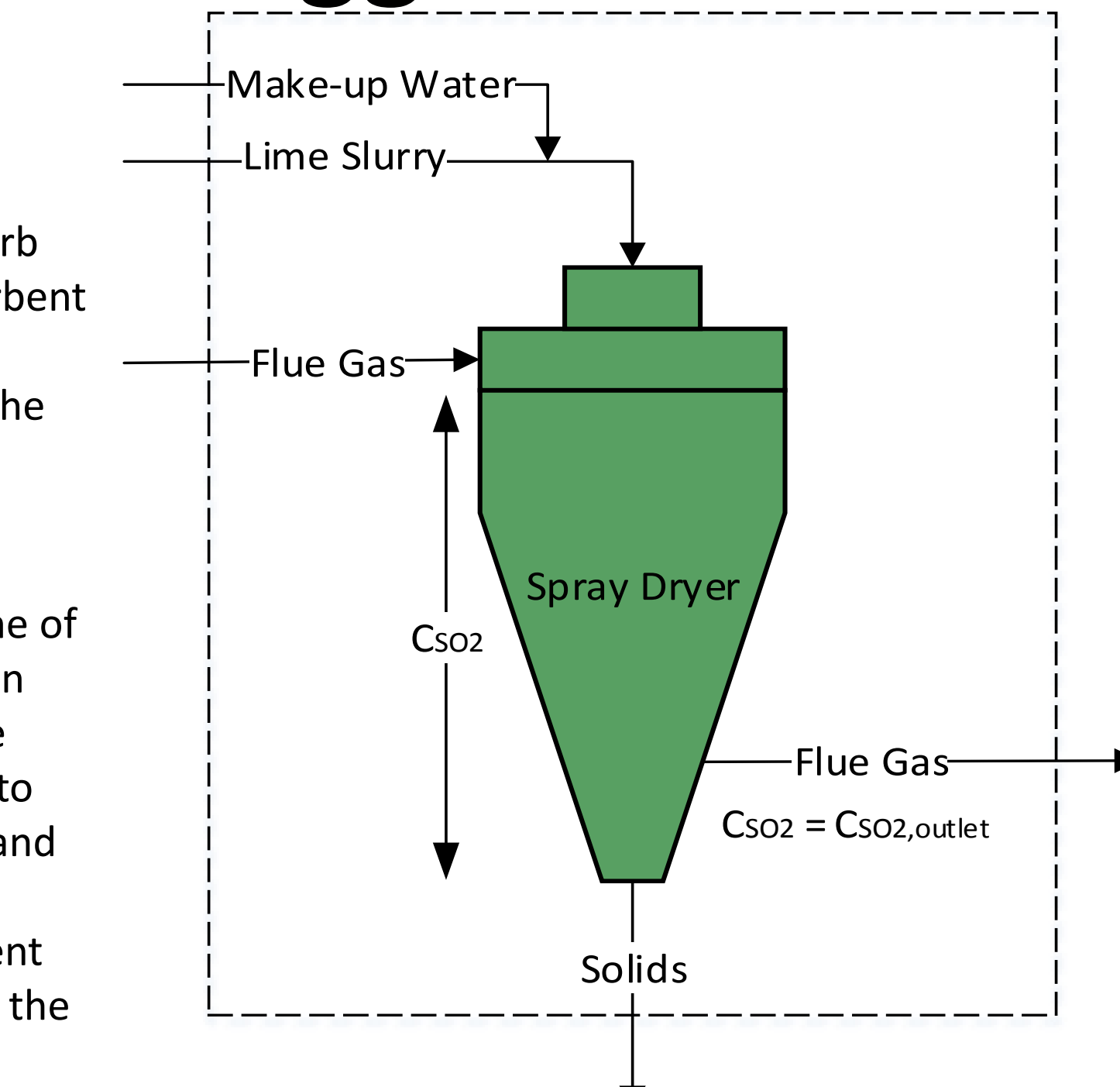


Figure 1: PFD of a Backmixed Spray Dryer

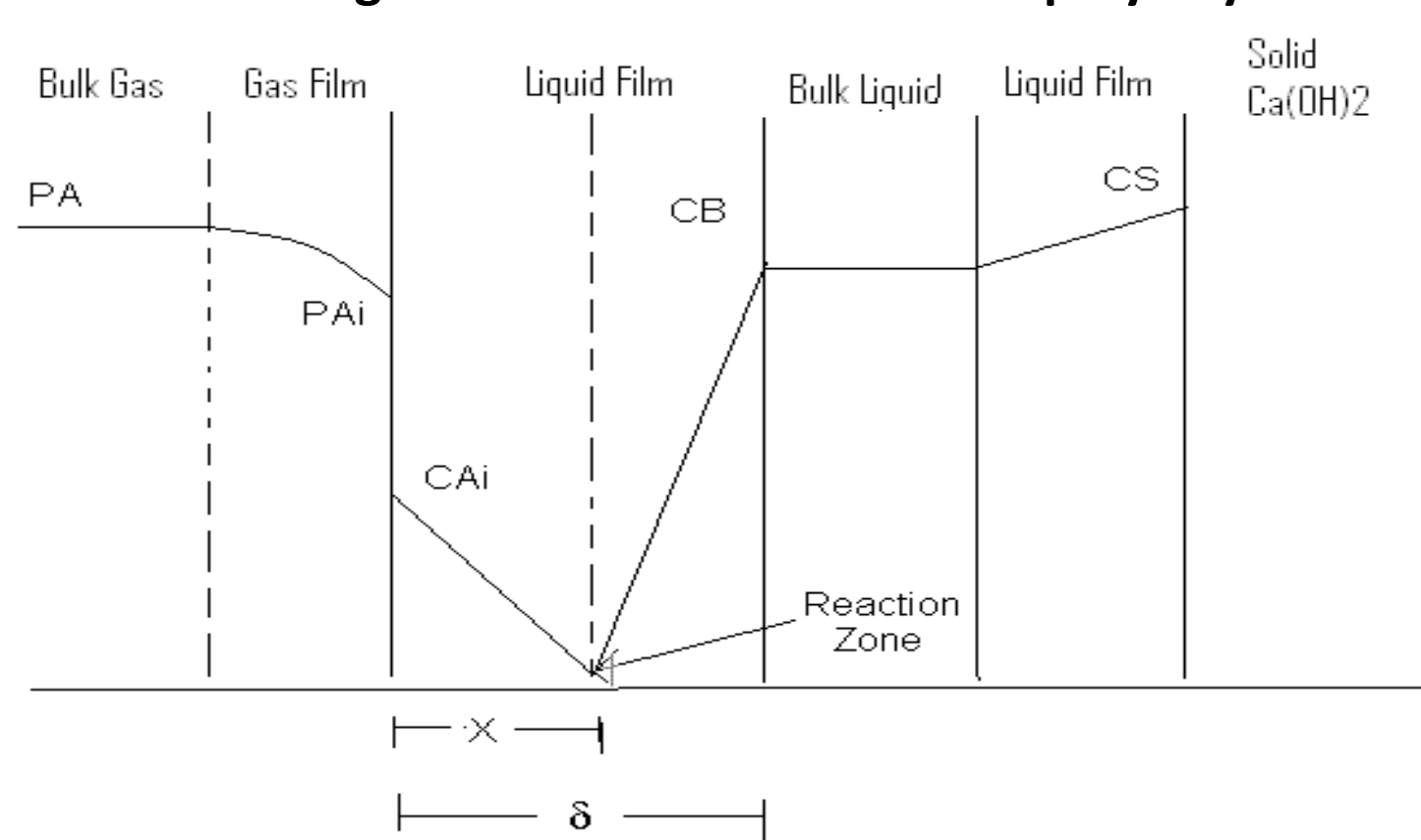


Figure 2: Concentration Profile of SO₂ and Ca(OH)₂

Constant and Falling Rate Period:

The first stage of droplet evaporation is known as the constant rate of drying period where the rate of evaporation is constant and dependent upon the mass transfer resistance to the transfer of water vapor by the gas film surrounding the droplet. The mass and heat transfer processes associated with this phase are as shown in **Figure 3**.

The second stage of droplet evaporation is the falling rate of drying which begins at the point at which the moisture content falls below the critical moisture content, which is the point at which the solid particles begin to touch one another within the slurry droplet. This in turn adversely affects its drying rate and causes the droplet diameter to stay constant given that the rate of drying is controlled by the diffusion of moisture through the slurry. The mass and heat transfer processes to be considered in this are shown in **Figure 4**.

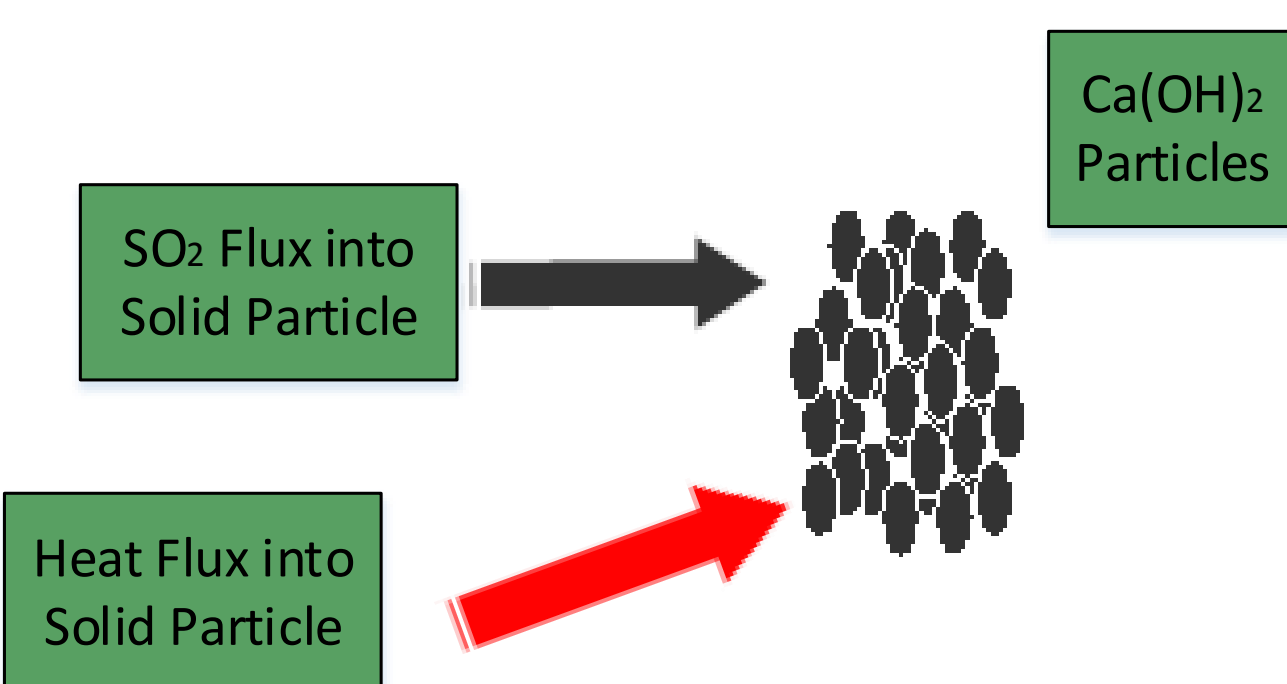


Figure 4: Processes Occurring Within a Slurry Droplet at the Falling Rate Period

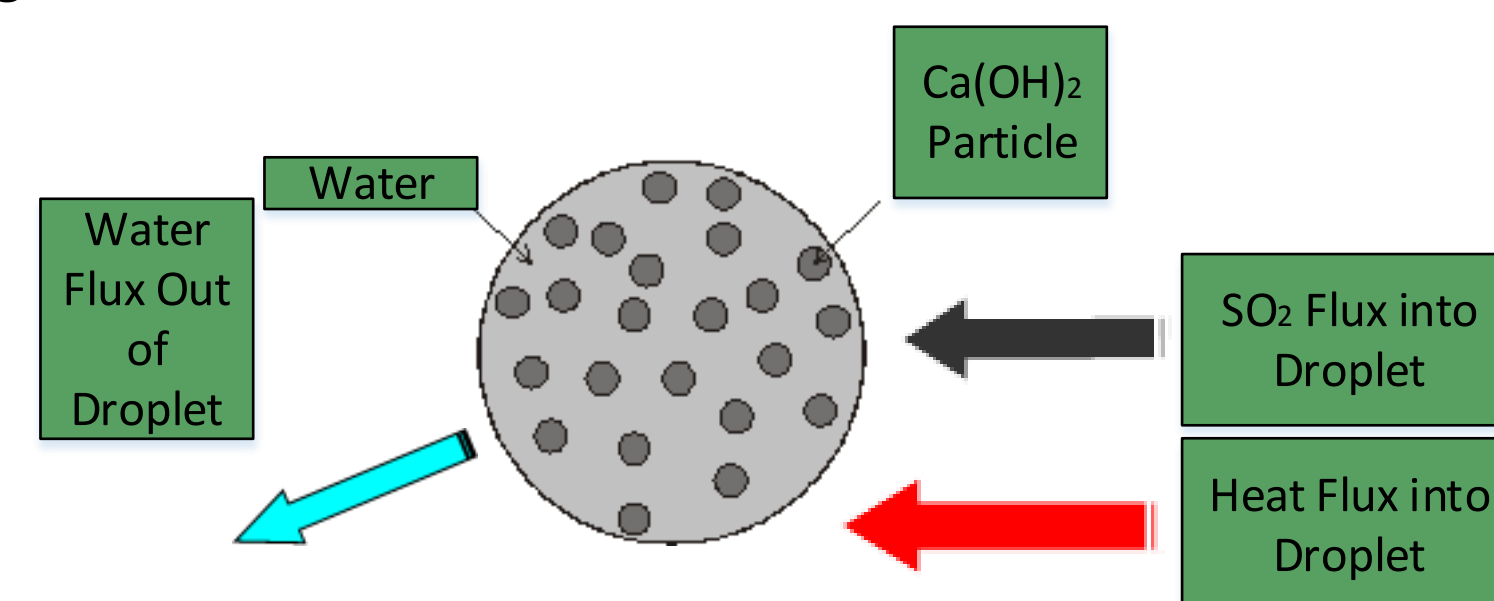


Figure 3: Processes Occurring Within a Slurry Droplet at the Constant Rate Period

Objective:

A Visual Basic program was developed that was capable of predicting the efficiency of a Backmixed Spray Dryer in terms of removing sulfur dioxide given the inlet conditions of the flue gas and lime slurry. A parametric study was then conducted in aims to properly characterize the inlet streams in an effort to optimize SO₂ removal efficiency.

Procedure:

A flowchart that summarizes logical steps taken to solve for the efficiency of a spray dryer with given inlet conditions is shown in **Figure 5**. The program itself can be divided into three different sections. The **first section** consists of providing the necessary inlet and operating parameters necessary for the program to calculate the efficiency of the reactor via spreadsheet format. The **second section** consists of the droplet phase and overall material and energy balances that are determined in order to establish the initial conditions of both the droplet and gas phase. These dependent variables are then initialized in order to conduct the **third section** of the program, which consists of solving the several differential equations that describes the behavior of the droplets. These ordinary differential equations are solved using a simple, explicit, finite forward difference scheme known as Euler's method. These derivative functions are determined at each time step, which in turn allows for the determination of the change in the droplet properties at each time step. Section 3 is reiterated until the efficiency solved for is found to be an acceptable value, or until there is either no more SO₂ that can be removed from the droplet or until the inputted estimated residence time of the droplet has been reached.

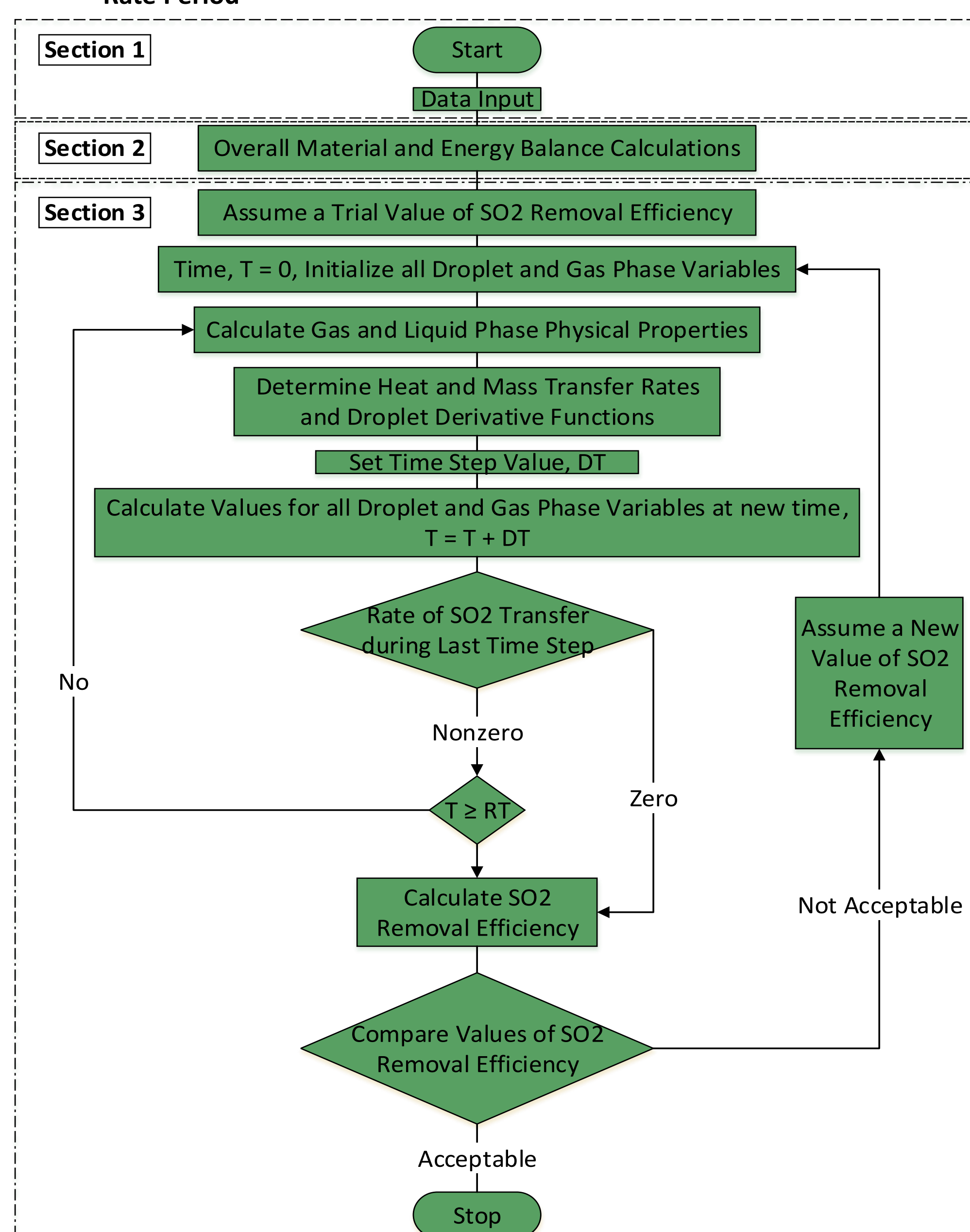


Figure 5: Logical Flowchart of the Computational Model of the Spray Dryer

Results:

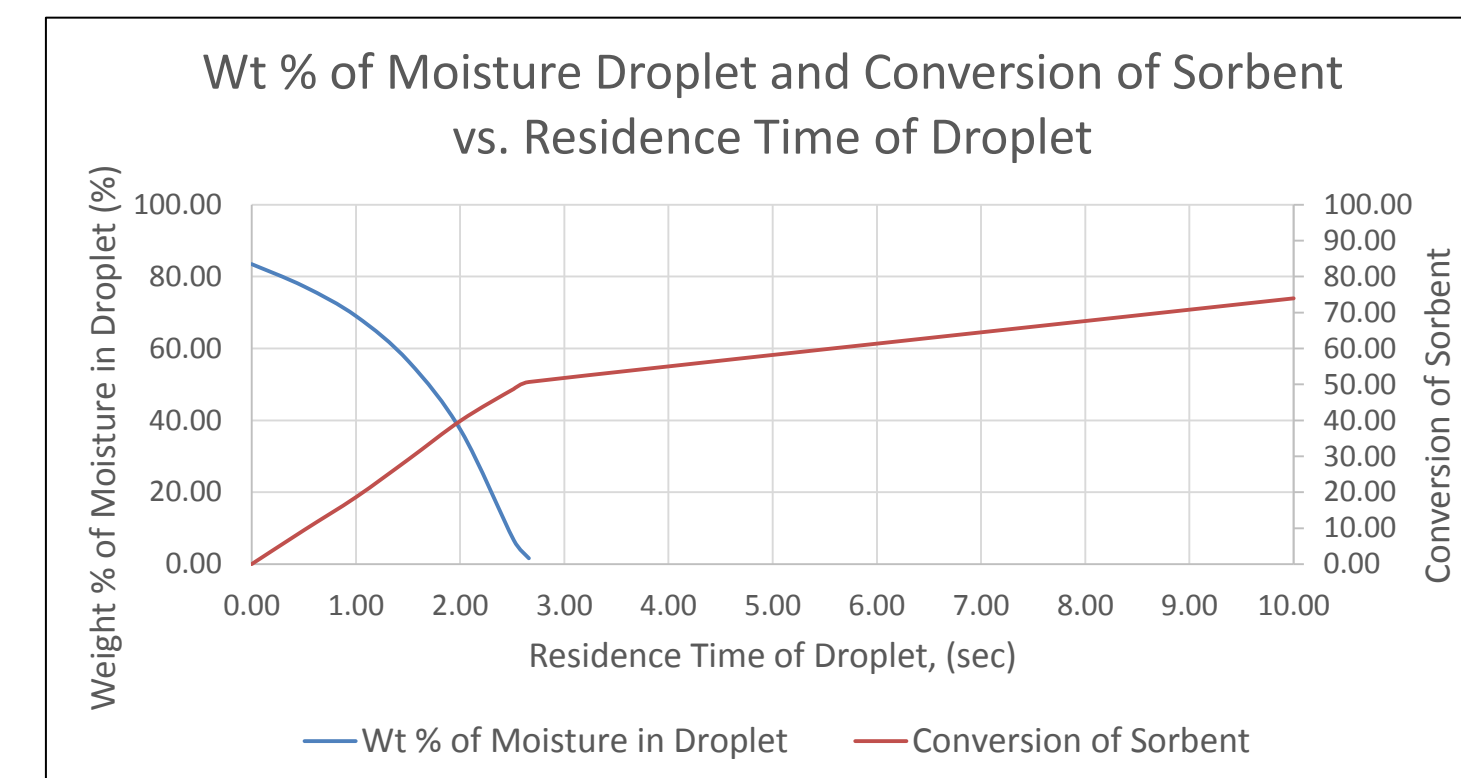


Figure 6: Weight Percent of Moisture in a Droplet and Conversion of Sorbent as a Function of Residence Time of a Droplet

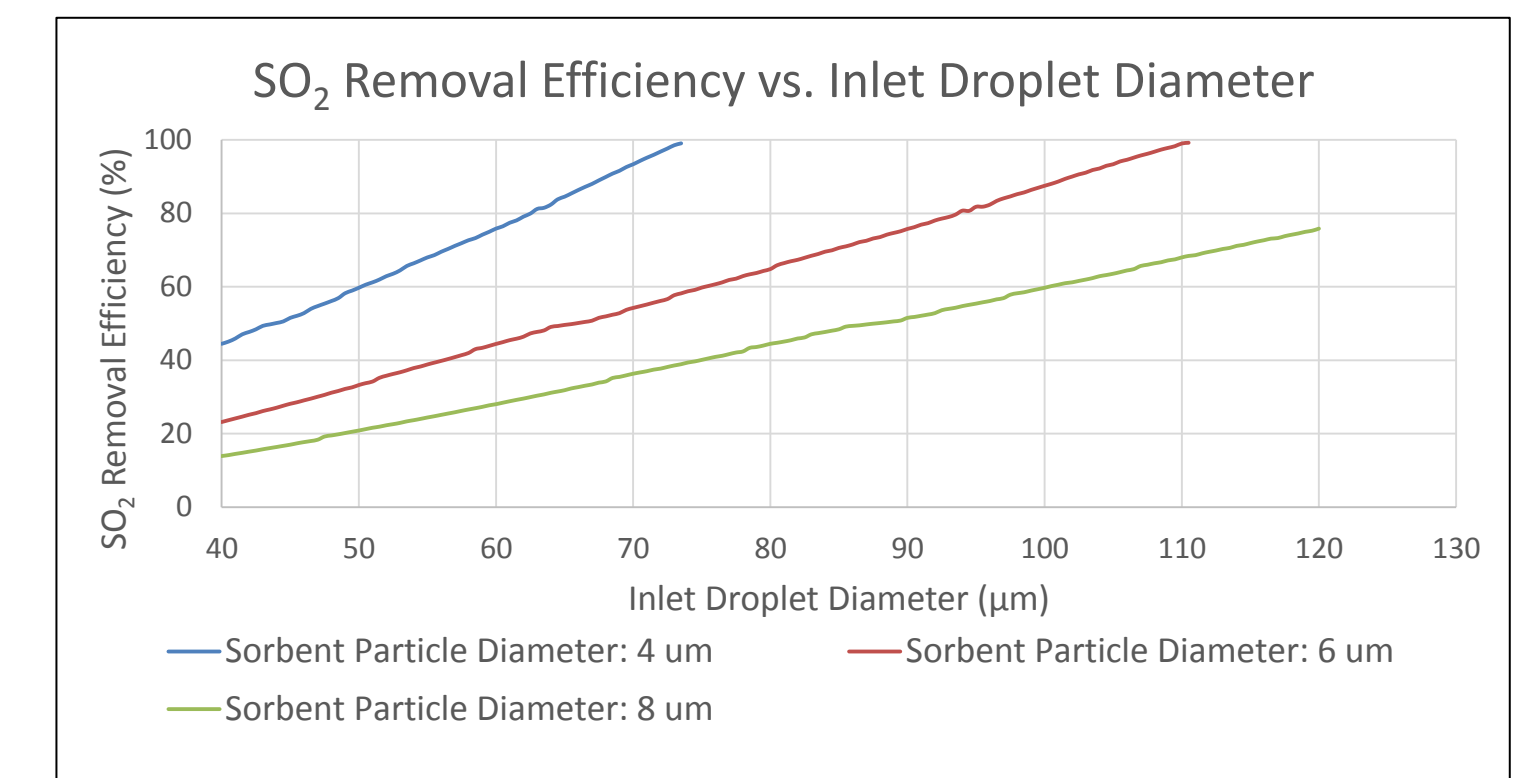


Figure 7: SO₂ Removal Efficiency as a Function of Inlet Droplet Diameter at varying Sorbent Particle Diameters

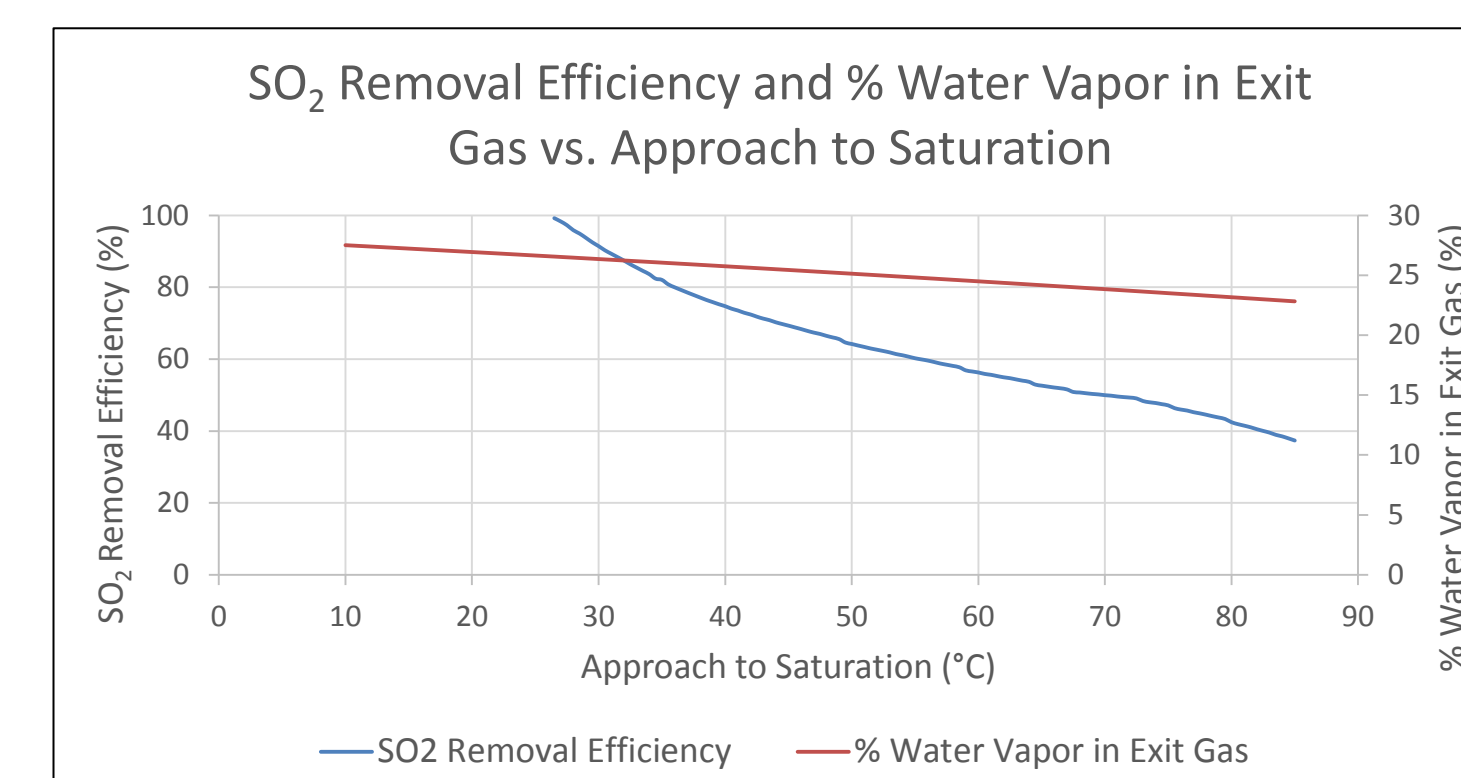


Figure 8: SO₂ Removal Efficiency and Mole Percent of Water Vapor in Exit Gas as a function of Approach to Saturation

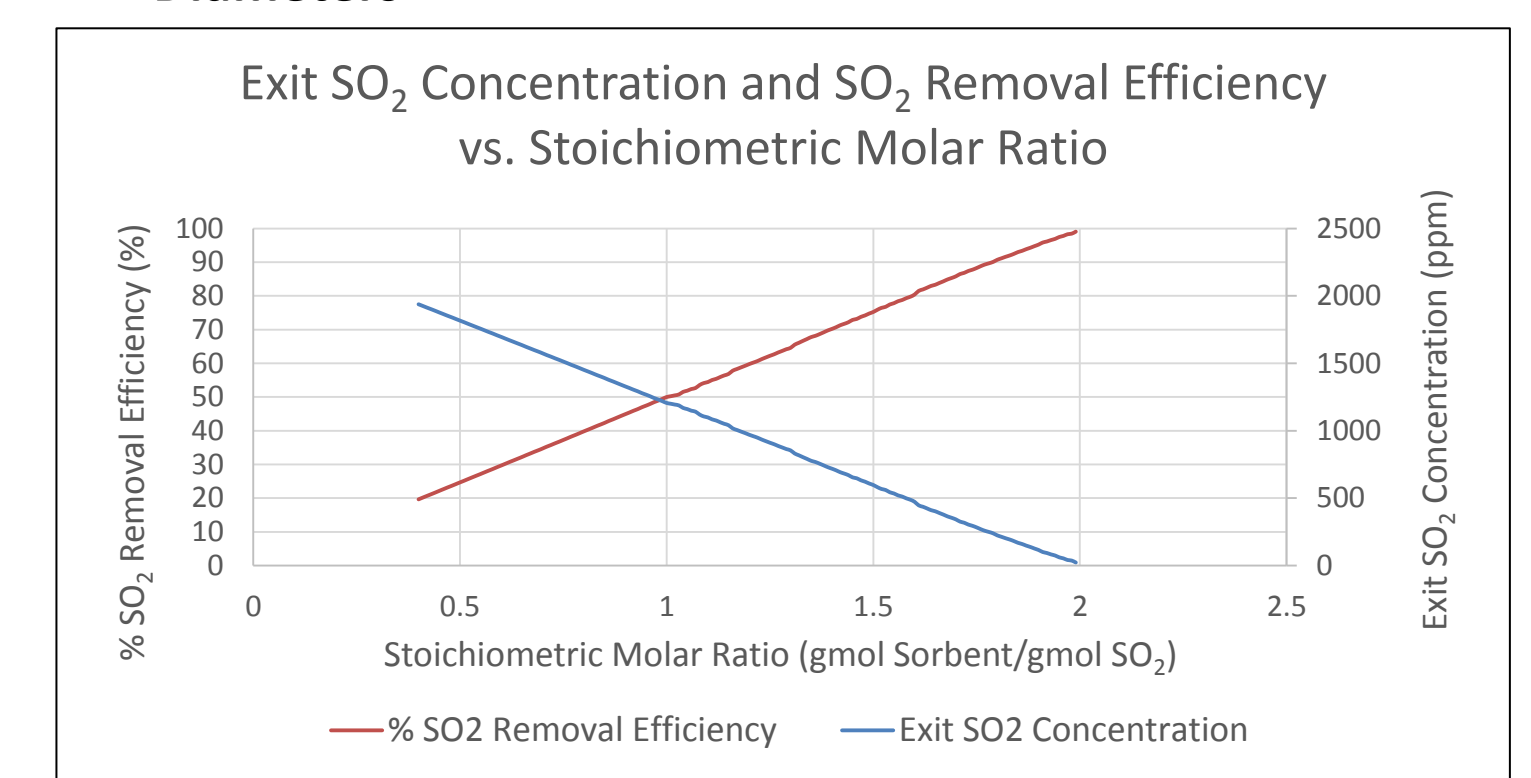


Figure 9: Exit SO₂ Concentration and SO₂ Removal Efficiency as a function of the Stoichiometric Molar Ratio

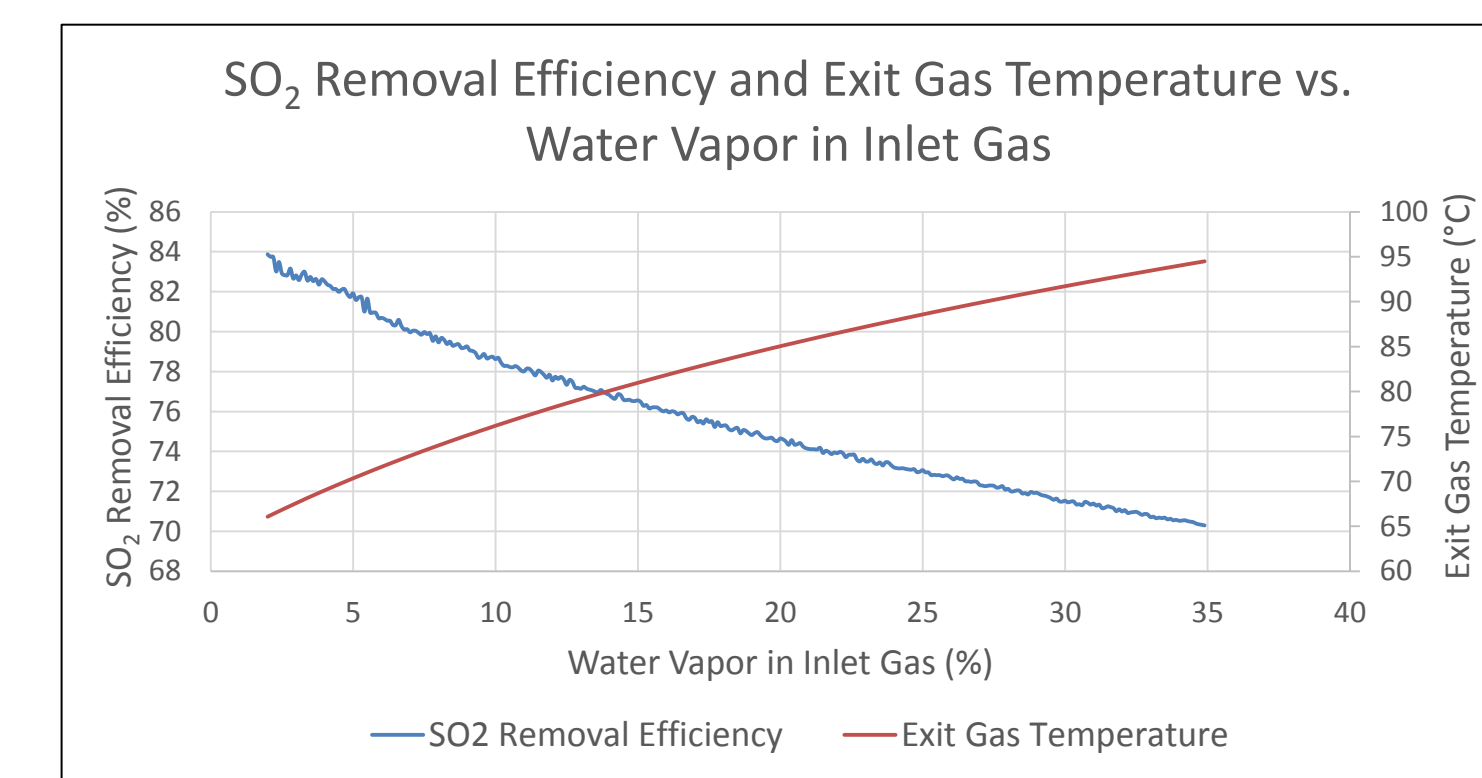


Figure 10: SO₂ Removal Efficiency and Exit Gas Temperature as a function of Mole Percent of Water Vapor in Inlet Gas

General Behavior

To gain a general understanding of the evaporation and absorption behavior of the spray drying process the weight percent of moisture of a droplet and the conversion of the sorbent as a function of residence time is shown in **Figure 6**. It is evident that the slurry droplet loses moisture within the first couple of seconds in the dryer as the moisture content reaches an equilibrium value. This 2-3 second period can be defined as the constant rate period. As most of the moisture is evaporated during this period, most of the SO₂ is absorbed during this period as well.

Parametric Study

A parametric study was conducted in order to observe and analyze the trends developed when varying key input variables to the whole process in order to gain a sense of what could be the optimal values of these variables that will allow further SO₂ removal. The key variables that are to be changed include Inlet Droplet Diameter, Sorbent Diameter, Approach to Saturation, Stoichiometric Molar Ratio, and Weight Percent of Water Vapor in Inlet Gas.

Figure 7 demonstrates that as inlet droplet diameter increases then the SO₂ removal increases as well. With an increase in droplet diameter there is a residual increase in the amount of water contained in a single droplet in the spray dryer and the presence of moisture enhances SO₂ absorption and the removal efficiency as mentioned before. Also, as you increase the sorbent diameter the SO₂ removal efficiency decreases because as the sorbent diameter is increased the sorbent particle surface area available for lime dissolution and in turn SO₂ absorption is reduced, therefore the removal efficiency of the spray dryer decreases.

In terms of approach to saturation, which is the difference between the outlet gas temperature and the wet bulb temperature, **Figure 8** shows that as the approach to saturation increases the SO₂ removal efficiency decreases and % water vapor in the exit gas decreases as well. Given that the approach to saturation is dependent upon how much makeup water is added to the spray dryer inlet, the lower the amount of water added leads to a reduction in the amount of water vapor in the exit gas and a reduction to the SO₂ removal efficiency due to the shorter constant rate period.

The stoichiometric ratio is known as the moles of calcium hydroxide fed to the system per mole of sulfur dioxide. **Figure 9** shows that as the stoichiometric ratio increases there will be an increase in the removal efficiency and based upon these results we can determine the amount sorbent that is needed to be added to achieve a certain removal efficiency by specifying the amount of SO₂ to be contained in the inlet gas.

The final key parameter of importance is the amount of water vapor in the inlet gas. As seen by **Figure 10**, SO₂ removal efficiency decreases when the amount of water vapor in the exit gas increases due to the fact that the initial presence of water vapor in the inlet gas provides significant resistance to SO₂ mass transfer to the droplet in the gas film phase. The exit gas temperature increases as well as an increase in the initial amount of water vapor also acts as a hindrance towards mass transfer of water vapor from the droplet to the bulk gas phase which was used to cool and humidify the flue gas.

Conclusion:

Based upon the results from the parametric study, it would be first be recommended to increase the droplet diameter while at the same time reducing the particle diameter as much as possible. It would also be recommended to reduce the adiabatic saturation temperature by increasing the amount of make-up water added initially. In terms of the stoichiometric ratio, it would be wise to maintain the ratio at a range of 1.9 to 2.1 in order to utilize the dryer at its maximum capacity for absorption while still leaving a residual amount of sorbent for further SO₂ removal. Finally, the amount of water vapor in the inlet gas should be minimized in order to diminish the mass transfer resistance in the gas film phase.

Future Work:

One recommendation for further study would be to compile experimental pilot plant data to further validate the results from this parametric study and to investigate the curvature of the trends noticed. To further improve the model, a surface area input for Ca(OH)₂ particles based upon experimental measurements can be implemented.