Educational Uses of COMSOL Multiphysics:
Carbon Dioxide Absorption with Chemical Reaction

A Major Qualifying Project Report:

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Submitted By:

Michael Morin

Approved:

William M. Clark, Advisor

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Abstract

Experimental procedures were developed to investigate an energy balance discrepancy between experimental data and theoretical predictions in a simple absorption system. Additional procedures were utilized to determine empirical correlations for mass transfer coefficients in a system with absorption and liquid phase chemical reaction. Data from both experiments was used to create a two-film model in COMSOL Multiphysics representing concentration profiles within an absorption and reaction system. Such a model will serve as a teaching aid allowing students to perform a virtual experiment when laboratory restrictions prevent them from investigating this type of absorption through conventional experimental methods.

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1 Introduction

Chemical absorption is a process that utilizes vapor-liquid equilibrium phenomena in order to separate one or more chemical species out of a gas phase by contacting the gas with a liquid in which the desired species can readily dissolve. This is a complex process that involves mass transfer within both the liquid and gas phases and transfer across phases through vapor liquid equilibrium.

For modeling purposes, it is convenient to group the various mass transfer parameters into overall mass transfer coefficients. One of the most typical formulations is to determine the overall mass transfer coefficient, $K_y a$, from overall gas and liquid phase mass transfer coefficients, $k_y a$ and $k_x a$, and through a Henry's constant,H representing the vapor-liquid equilibrium.

$$\frac{1}{K_y a} = \frac{1}{k_y a} + \frac{H}{k_x a}$$

This overall mass transfer coefficient can then be used to implement a lump parameter model in which both phases are treated as continuums with mass appearing or disappearing through vapor-liquid equilibrium all throughout the body of the system.

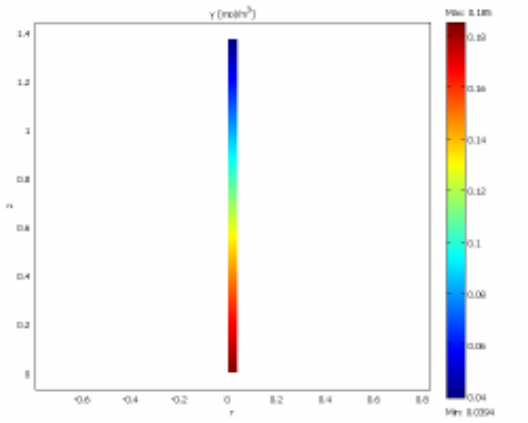

Figure 3: Lumped Parameter Model output for simple absorption

Alternatively, the individual parameters from the overall mass transfer coefficient equation can be used separately to create a two-film model. The gas and liquid side coefficients govern the movement of mass through the central stagnant boundary layers while the Henry's constant governs the transfer across the boundary.

Unfortunately, some species do not have high enough solubility in water for simple absorption to be a viable option. In this particular investigation, the absorption of carbon dioxide from air into liquid water will be considered. This is one such systems with limited solubility.

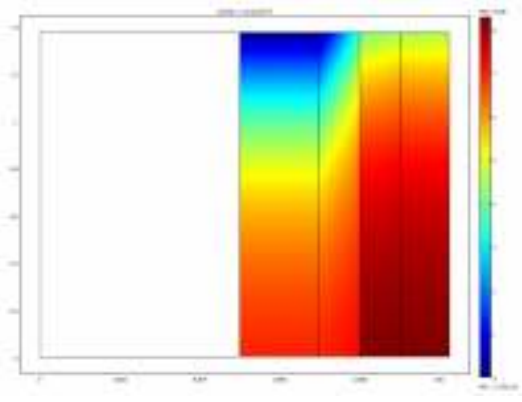

Figure 4: Two-film model output for simple absorption

Since CO_2 removal from waste gas streams is an important topic in industrial applications, alternative methods must be developed. One practical way to increase the

removal of CO_2 from the gas stream during absorption is to add sodium hydroxide to the liquid phase. Once the carbon dioxide absorbs, it undergoes reaction with the aqueous hydroxide ions to form a highly soluble product ion.

$$CO_2 + 2OH^- \longrightarrow CO_3^{2-} + H_2O$$

Although students study simple absorption during their course of study as chemical engineers, this enhanced form of absorption is difficult to demonstrate in a class room setting and is often not included in the curriculum. It would be useful to develop a tool for studying this type of absorption without the need for physical laboratory equipment. The remainder of this report represents an effort to fulfill this goal.

2 Objective

The objective of this project is to develop an interactive teaching aid that will allow students to investigate the internal dynamics of an absorption column when it is operated in conjunction with a liquid phase chemical reaction. Such an aid will allow students to virtually experiment with this advanced method of absorption without the need to perform the physical experiment. Since the physical experiments for this type of system are generally too dangerous and difficult to implement in a laboratory based class setting, students currently are unable to explore this important process without this teaching aid.

Furthermore, this teaching aid will be developed using COMSOL Multiphysics software. This program is a powerful finite element package that combines mesh generation tools, solution solvers, and postprocessing tools. By establishing a model, students will then be able to enter the program and adjust specific parameters. By doing this, they can study the system's response to various types of variable manipulations.

3 Methodology

To fulfill the project's goal; it was useful to break the overall objective into a series of smaller tasks. Each of these tasks addresses a specific topic of interest necessary to create the final teaching tool.

1. To resolve an energy balance discrepancy for the simple carbon dioxide absorption models
2. To collect data from an absorption column running with aqueous sodium hydroxide liquid phase to induce chemical reaction
3. To model an absorption column running with aqueous sodium hydroxide liquid phase to induce chemical reaction

The first task is to address a known issue with the energy balance for the simple of CO_2 in water. Carbon dioxide absorption into water is a known exothermic reaction: ΔH_s=-*20.3kL mol*$^{-1}$[1]. Assuming no other significant heat effects are occurring, the liquid phase should gain heat as it flows through the absorption column. In direct conflict with the theory, experimental data from the Goddard Hall's pilot scale column indicate a 10 ˚F temperature drop between the liquid inlet and outlet. This is a substantial change in temperature and would indicate that an important physical phenomenon is missing from the simple models. Before a more complex absorption/reaction model could be developed, this energy balance discrepancy needed to be resolved.

Next, data must be obtained for a column operating under the conditions of interest. While published experimental data would be suitable, it was decided that by collecting an independent set of data it would be possible to a much greater degree of control over the dependant parameters of the system. Unfortunately, the aspects of this experiment that make it difficult to perform in a laboratory based class setting also make it difficult in general within an academic institution. To overcome these difficulties, a mini absorption column had to be built and then operated in order to obtain the desired data.

Finally, once experimental data had been made available, it could be used to develop the teaching aid. Since it is difficult to determine analytically the system's mass transfer parameters, the data was used to fit these parameters. Doing this over a range of liquid flow rates, empirical correlations for the mass transfer parameters could be developed for use in the models.

[1] M Taghizadeh et al. *Chemical Engineering Journal* **82** (2001) 143-148.

3.1 Resolving the Energy Balance Discrepancy for Simple Absorption Models

The two most likely causes for the decrease in liquid phase temperature across the column include non isothermal expansion of the gas phase at the base of the column and heat loss due to evaporation.

As the gas phase enters the column, it emerges from a narrow tube into a much wider column. This rapid expansion is usually accompanied by a decrease in temperature. If this heat effect is strong enough, it could be causing the liquid to cool enough to overcome the heat of absorption.

Alternatively, the liquid phase could be evaporating into the gas phase. The gas used for these experiments comes from compressed gas cylinders which contain no humidity. As this dry gas comes in contact with the air some of the liquid will evaporate in order to humidify the gas until it becomes saturated with water vapor. Since evaporation is an endothermic process, if sufficient evaporation is occurring, it could overcome the heat of absorption.

3.1.1 Experiment #1: Non-Isothermal Expansion

3.1.1.1 Objective

To determine the degree of cooling occurring due to isothermal expansion of the gas phase

3.1.1.2 Equipment

- Goddard Hall Pilot Scale Packed Absorption Tower with peripheral flow controls, flow meters, and thermo couples
- Compressed air cylinder
- Compressed carbon dioxide cylinder

3.1.1.3 Procedure

For this relatively simple experiment, the column was operated using only a gas phase. Gas flow rates were adjusted to maintain a constant 1.5 LPM flow of air and 0.3 LPM flow of carbon dioxide. The system was allowed to run while temperature measurements were taken at the top and bottom of the column

3.1.2 Experiment #2: Evaporation Heat Loss

3.1.2.1 Objective

To determine if saturating the gas phase with water vapor prior to its use in the column will prevent the liquid phase temperature drop.

3.1.2.2 Equipment

- Goddard Hall Pilot Scale Packed Absorption Tower with peripheral flow controls, flow meters, and thermo couples
- Rosemont carbon dioxide analyzer
- Compressed air cylinder
- Compressed carbon dioxide cylinder
- Pressure vessel with appropriate fittings and tubing
- Water

For this experiment, the gas inlet tubes to the column were rerouted. After the junction where the two gas streams are mixed, the gas was diverted into a pressure vessel. At the inlet of the vessel, the gas is forced down a vertical, internal tube to emerge at an orifice located near the bottom of the vessel. A second opening at the top of the pressure vessel was used as an outlet. Gas emerging from this outlet was then piped into the column.

3.1.2.3 Procedure

To ensure that the water supply to the column remained constant throughout the experiment, the liquid hold-up tank was first drained of its room temperature water and then refilled using the buildings water supply which was slightly colder than room temperature. Thus, as the holding tank refilled during the experiment, it would not decrease in temperature.

Next the pressure vessel was filled with water from buildings water supply and then sealed. Once sealed, the gas cylinders were opened and set to flow at cost rates of 1.5 LPM air and 0.3 LPM CO_2. With the addition of the pressure vessel, the gasses were now being bubbled through a water bath before entering the tower. Since the gas would now be saturated with the water from the tank and not from the flowing water in the column, there should no longer be a temperature drop across the column.

A liquid flow rate of 1 LPM water was used and measurements were taken over a period of time once the outlet gas CO_2 concentration had reached a steady state.

3.1.3 Experiment #3: Control Case

3.1.3.1 Objective

To analyze the column as it operates under the typical laboratory conditions in order to determine if some other phenomena may be occurring.

3.1.3.2 Equipment

- Goddard Hall Pilot Scale Packed Absorption Tower with peripheral flow controls, flow meters, and thermo couples
- Rosemont carbon dioxide analyzer
- Compressed air cylinder
- Compressed carbon dioxide cylinder
- Water

For this experiment, the pressure vessel was left attached to the column; however the water bath was drained. Effectively, the column set-up as it would be during the laboratory experiments. The addition of the empty pressure vessel merely increased the pressure drop over the system without effecting compositions or temperature.

3.1.3.3 Procedure

To ensure that the water supply to the column remained constant throughout the experiment, the liquid hold-up tank was first drained of its room temperature water and then refilled using the buildings water supply which was slightly colder than room temperature. Thus, as the holding tank refilled during the experiment, it would not decrease in temperature.

The column was then run using a standard set of conditions encountered during a typical experiment: 1.5 LPM air, 0.3 LPM CO_2, and 1.0 LPM water. In addition to recording the digital readouts from the thermocouples, the temperature of the liquid in the hold up tank was manually collected using a thermometer.

3.2 Collecting Data from an Absorption/ Reaction System

3.2.1 Obstacles

As previously mentioned, there are many obstacles that must be overcome to run an absorption with reaction experiment in an academic setting.

First and foremost, the aqueous sodium hydroxide[2] to be used as the liquid phase has a pH of 14. This is extremely hazardous to humans. Contact with the skin, eyes, or lungs and ingestion can all cause sever burns and scaring. Permanent vision loss, scaring, and even death can occur if this solution is handled inappropriately. Additionally, pH 14 substances can also be corrosive when they come in contact with inorganic material. Liquid flowing through the Goddard Hall absorption column comes in contact with a wide variety of materials including glass packing, gaskets, plastic tubing, metal fittings, flow meters, and pumps. Any one of these pieces could easily react with the sodium hydroxide causing permanent damage to the system.

Of lesser concern is the volume of aqueous sodium hydroxide required. The system requires at least 20 minutes, if not longer, to reach steady state. Even running at the minimum measurable flow of 0.5 LPM liquid, the volume of liquid required is substantial. To complicate the matter more, the hold-up tank requires a minimal liquid level in order to provide net positive suction head (NPSH) to the pump. Therefore a secondary liquid hold-up tank would need to be designed in order to gravity feed the first hold-up tank and maintain NPSH.

Finally, initial modeling using known reaction kinetics indicated that, under the normal operating conditions, carbon dioxide would be rapidly depleted from the gas phase shortly after entering the column. Since the available equipment can only measure concentration at the inlet and outlet, all data points would be identical over the normal range of system parameters. In other words, no useful data could be achieved from the column using standard operating conditions. Theoretically, this could have been overcome by greatly increasing the gas flow rate

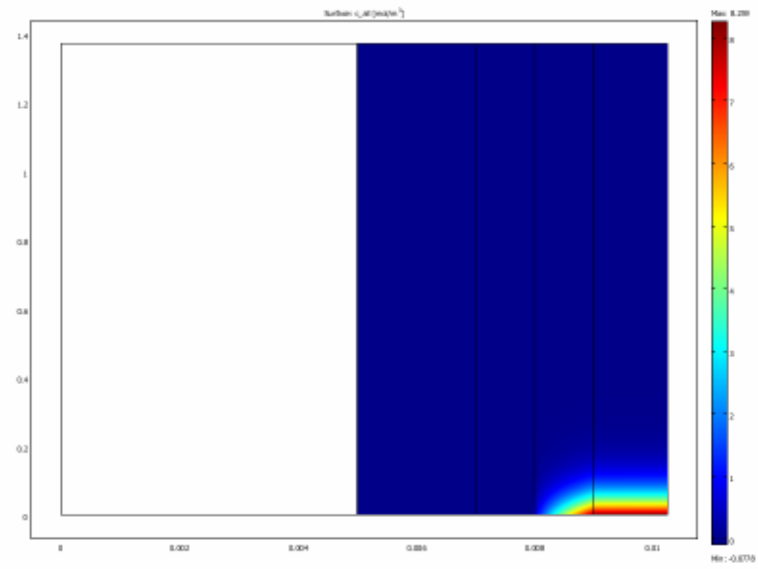

Figure 5: Predicted concentration profile for absorption with reaction within the Goddard Hall column operating under standard lab conditions.

[2] See the appendix for a full MSDS for sodium hydroxide

while decreasing the liquid flow—essentially contacting more CO_2 with less liquid in hopes of some of the CO_2 remaining at the outlet. However, this method has its own inherent issue. The flow meters on the system would have to be replaced since the current meters would not be sensitive enough to fine tune the liquid flow rate and the high gas flows would physically damage the gas flow meters.

Overall, among the safety issues for humans and equipment, the high volume of solution required, and the inability to obtain usable data, it became apparent that using the Goddard Hall pilot scale column would be completely impractical. Instead, it was decided to create a miniature absorption column that could be operated under more favorable conditions. Although the safety issues still remained, this new approach negated the latter two concerns.

3.2.2 Equipment

- 1.75" ID Acrylic Tube, 15" in length
- 2, 2-hole rubber stoppers
- Metal disk with holes and legs
- Stand with clamps
- Glass packing material
- Tubing and appropriate fittings
- Peristaltic Pump
- Adjustable Pump Controller
- 2 Large Plastic liquid container
- Gas feed and meters from Goddard column
- 1000 mol/m^3 NaOH in H_2O solution
- Rosemont carbon dioxide analyzer
- Rubber Gloves
- Eye Protection

Figure 6: Miniature absorption column used in data collection for absorption/reaction system

By using similar materials to those found in the Goddard hall column, it was possible to construct a miniature column with dimensions of 1.75" diameter and 12.75" height. The gas input was line was transferred directly from the Goddard column to the miniature column. With this, the same setting of 1.5 LPM air/0.3 LPM CO_2 could be easily achieved using the flow control equipment from the original column. Even though the same volumetric flow rate was used for both absorbers, the mini-column's smaller cross sectional area resulted in a much higher superficial velocity, as was desired.

To control the liquid, a peristaltic pump was used to pump liquid from hold-up container into the column. Since the pump was controlled by an adjustable control device, experiments would be needed to calibrate the controller settings to actual flow rates.

3.2.3 Experiment #4: Liquid Flow Rates

3.2.3.1 Objective

To correlate the adjustable controller's settings to the actual liquid flow rates.

3.2.3.2 Equipment

- Peristaltic Pump
- Adjustable Pump Controller
- Tubing
- Stop Watch
- 250 mL graduated cylinder

Figure 7: Adjustable Control on Pump Control Device

3.2.3.3 Procedure

Setting the controller to an incremental value between 2 and 6 inclusive, the pump output was collected in the graduated cylinder for a fixed period of time. Thus the liquid volumetric flow rate could be determined. Unfortunately, the controller was continuous and could be set at any position between two intervals. This allowed for the possibility that each time it was set to a specific number, it may have been slightly different than the previous time. Since nothing could be done about this flaw, the small amount of error that it introduced will have to be acceptable.

3.2.4 Experiment #5: Simple Absorption in Mini-Column

3.2.4.1 Objective

To obtain data for simple absorption in the mini-column that can be used to determine fitted overall mass transfer coefficients.

3.2.4.2 Equipment

- Miniature column and pump assembly
- Rosemont carbon dioxide analyzer
- Air and carbon dioxide
- Distilled water

3.2.4.3 Procedure

The column was run with a fixed gas flow rate of 1.5 LPM air/ 0.3 LPM CO_2. Liquid flow rate was adjusted from setting 2 to setting 6 (0.136 to 0.4 L/min). At each liquid flow, the column was allowed to run until exiting gas phase CO_2 concentration reached steady state for at least 1 minute. Liquid output was captured in a plastic jar and disposed of after the experiment.

3.2.5 Experiment #6: Absorption/Reaction in Mini-Column

3.2.5.1 Objective

To obtain data for absorption/reaction in the mini-column that can be used to develop the absorption/reaction model.

3.2.5.2 Equipment

- Miniature column and pump assembly
- Rosemont carbon dioxide analyzer
- Air and carbon dioxide
- 1000 mol/m^3 NaOH solution

3.2.5.3 Procedure

NaOH solution was prepared by adding 40 grams of NaOH pellet per liter of water. Pellets were slowly dissolved into a portion of the water using a stirring rod. The final solution was then diluted to the proper volume. NaOH solution sat at room temperature for an hour before experiments were performed.

The column was run with a fixed gas flow rate of 1.5 LPM air/ 0.3 LPM CO_2. Liquid flow rate was adjusted from setting 2 to setting 6 (0.136 to 0.4 L/min). At each liquid flow, the column was allowed to run until exiting gas phase CO_2 concentration reached steady state for at least 1 minute. Liquid output was captured in a plastic jar and disposed of after the experiment.

3.2.5.4 Safety

Latex gloves and safety glasses were worn at all times when handling NaOH. NaOH container was clearly labeled and stored on sturdy surfaces. Unnecessary personal were asked to keep their distance from the equipment during operation.

Waste NaOH was first diluted before flushing down a chemical drain. Equipment was thoroughly and repeatedly rinsed with fresh water. Solid material found trapped in chemical drain was thoroughly washed and disposed of in appropriate receptacle. pH tests were performed on all equipment pieces to ensure pH neutrality before leaving the laboratory.

3.3 Modeling Absorption/ Reaction System

3.3.1 Overall Mass Transfer Coefficient

For the lumped parameter model, two differential equations are used: one for the liquid phase and on for the gas phase CO_2.

$$\nabla \cdot (-D\nabla c) = R - u \cdot \nabla c$$

Using known diffusivities for carbon dioxide in water and air[3] and the experimentally set flow rates, the only remaining parameter is the reaction term R. In the liquid phase

$$R = K_y a \cdot (y - y^*)$$

representing an overall transfer of mass into the liquid phase. Simultaneously, this mass must be removed from the gas phase, so

$$R = -K_y a \cdot (y - y^*)$$

Determining y^* by means of Henry's Law, the overall mass transfer coefficient, $K_y a$ is the only tunable parameter in the lumped model. Setting the correct inlet concentrations, the $K_y a$ parameter can then be adjusted for each flow rate in order to find a the value that will yield the correct outlet concentration. In this way an empirical correlation can be determined to find the overall mass transfer coefficient given various liquid flow rates.

3.3.2 Gas Phase Mass Transfer Coefficient

By modifying the lumped parameter model slightly, it can be easily adapted to incorporate a liquid phase chemical reaction. In fact, in terms of the CO_2 balances, the only change needed is to add a consumption term to R:

$$R = K_y a \cdot (y - y^*) - k_b C_{CO_2} C_{OH^-}$$

The only complication is that additional mass balances must also be added to track not only the OH^- concentration, but also the Na^+ and CO_3^{2-} concentrations since the reaction rate constant is dependant on these ionic concentrations. From the literature[4], an empirical correlation can be found for this constant:

$$\log(k_b) = 11.895 - 2382/T + 0.221I - 0.016I^2$$

Where "I" is the ionic strength of the solution and T can be taken as room temperature.

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[3] Clark, W. M. "COMSOL Multiphysics Models for Teaching Chemical Engineering Fundamentals: Absorption Column Models and Illustration of the Two-Film Theory of Mass Transfer." 2008.

[4] M. Taghizadeh et al. *Chemical Engineering Journal* 82 (2001) 143-148

After making these modifications to the model, it was seen that very little reaction was occurring, indicating an error in the model. It was soon realized that, by using the overall mass transfer coefficient from a system without reaction, the model was artificially imposing a liquid phase mass transfer resistance. Since the reaction had been added specifically to remove this barrier to mass transfer, it is wrong to use the overall mass transfer coefficient. Instead, only gas phase mass transfer coefficient should impact the system.

$$\frac{1}{K_y a} = \frac{1}{k_y a} + \frac{H}{k_x a} \cong \frac{1}{k_y a} = H_y$$

Once again, but adjusting the mass transfer coefficient, a correlation can be developed between liquid flow rate and overall gas phase mass transfer coefficient, $k_y a$. The validity of this equation can be tested by comparing the results to known correlations[5]:

$$H_y = \left(\frac{0.226}{f_p}\right)\left(\frac{Sc}{0.660}\right)^{0.5}\left(\frac{G_x}{6.782}\right)^{-0.5}\left(\frac{G_y}{0.678}\right)^{0.35} = C\left(\frac{G_x}{6.782}\right)^{-0.5}$$

Here f_p is an unknown packing parameter, Sc is the Schmidt number, and G_x and G_y are liquid and gas phase superficial velocities respectively. Since everything except the liquid phase superficial velocity is constant for these experiments, it can be seen that a correlation to the gas phase mass transfer resistance, H_y, should be directly proportional by some constant C, to G_x raised to the inverse, one-half power.

3.3.3 Two-Film Absorption with Reaction Model

Using known rate constant, diffusivities, and Henry's constant in addition to the empirical correlations for mass transfer coefficients, the two-film model is easily adapted to reflect absorption with chemical reaction. The correlation for the overall gas phase mass transfer coefficient is used directly in the model to predict the CO_2 behavior in the stagnant gas film. Within the stagnant liquid film, the overall mass transfer coefficient is set to an arbitrarily large value to ensure that the liquid phase resistance to mass transfer is close to zero. Finally, reaction terms are added to both the stagnant liquid film and the falling liquid layer in order to account for the removal of CO_2 by chemical reaction. As with the lumped parameter model, extra differential equations were added to track the liquid phase ion concentrations.

[5] Geankoplis. *Transport Processes and Separation Process Principles*. Prentice Hall: Upper Saddle River, NJ, 2003

4 Results

4.1 Resolved the Energy Balance Discrepancy for Simple Absorption Models

4.1.1 Experiment #1: Non-Isothermal Expansion

After a period of about 45 minutes, the bottom of the column was approximately 12 ˚F cooler than the top of the column. This suggests that there is in fact cooling occurring due to the non-isothermal expansion of the gas phase.

Table 1: Temperature data (˚F) collected at intervals over a 45 minute period

Top	Bottom
77	73
77	71
77	65

However, this similarity in temperature drop does not correspond to an equivalent heat loss. The heat capacity of air in this temperature range is approximately 1.00 kJ/kg*K while the heat capacity of water is approximately 4.18 kJ/kg*K[6]. Taking into consideration the density of air and water (1.17 kg/m^3 and 1000 kg/m^3 respectively)[7], a 12˚F temperature drop in the gas would correspond to the gas absorbing 7.8 kJ/m^3 of heat. For the liquid to supply this heat, its temperature would only fall by 0.003 ˚F.

Clearly, non-isothermal expansion is not responsible for the temperature drop across the column. While this experiment demonstrated that there was indeed cooling due to this phenomena, it is so insignificant that it can be neglected from the overall model without incurring significant error

4.1.2 Experiment #2: Evaporation Heat Loss

After allowing the column to approach steady state, there was a 12˚F temperature drop over the column despite the addition of the humidification system. This indicates that while there may be evaporation and cooling occurring within the standard system, it is not causing the overall discrepancy with the energy balance.

Table 2: Temperature data (˚F) for column with preconditioned gas phase

Top	Bottom
68	55
67	55

Table 3: Temperature data (˚F) for column under standard conditions

Top	Bottom
72	74
72	66
70	58
70	58
69	57

4.1.3 Experiment #3: Control Case

By performing the experiment under the standard conditions, it was possible to reproduce the 12˚F temperature drop across the column. However, measurement of the water in the liquid hold-up tank showed it to be approximately 54.5˚F. This is significantly cooler than the temperature at the top of the column. While the liquid pump does add a small amount of heat to the liquid to get it to the top of the column, it does not add 15˚F. It is therefore likely that the temperature of the water at the top of the column is actually closer to 55 or 56˚F.

[6] Incropera, Dewitt, Bergman, and Lavine. *Introduction to Heat Transfer*. 5th ed. John Wiley & Sons: USA, 2007.
[7] ibid

Likely, the thermocouple at the top of the column is either inappropriately positioned or malfunctioning. If the top thermocouple is not adequately contacting the liquid phase then it will not give an accurate reading of the liquid phase temperature. To correct this, the thermocouple would need to be placed either directly under the liquid phase inlet so that the liquid would fully coat the thermocouple or the thermocouple should be placed within the liquid phase input pipe. Alternatively, if the thermocouple is accurately placed, it could just be malfunctioning and needing replacement.

In light of these results, it can be seen that there actually is not a discrepancy in the energy balance. The system is consistent with the theory being applied. It was merely an in appropriately interpreted temperature reading that was causing confusion.

As an unexpected result, the new data showed that system was only experiencing a temperature increase of less than 1 or 2˚F. Since the mass transfer parameters are not highly sensitive to temperature changes, this experiment showed that it was not necessary to include the energy balance in the teaching aid. This will significantly reduce the complexity of the tool, making it easier for students to understand.

4.2 Collecting Data from an Absorption/ Reaction System

4.2.1 Experiment #4: Liquid Flow Rates

By collecting the output for 30sec or 1 min at each setting, it was possible to generate a table correlating the controller settings to actual liquid flow rates. As expected, the flow rate increases with increase setting, but it is not a linear relationship: Flow increases slower as setting increase. Again this could have some error due to the inability to set the controller in exactly the same spot each time. Also, as the tubing inside the pump began to physically deteriorate due to the stresses, it could have affected the flow rate.

Table 4: Flow rate vs. Controller Setting

Setting	W(L/min)
off	0
2	0.136
3	0.23
4	0.284
5	0.348
6	0.4

4.2.2 Experiments # 5 & #6: Simple Absorption and Absorption/Reaction Data Collection

Both experiments produced well behaved data sets. Both appropriately exhibited decreasing linear trends. As expected, the simply absorption experiment showed poor removal of CO_2 from the gas stream. With an inlet concentration of 17.5 mol-%, the highest water flow rate only decreased the CO_2 by 1.4 mol-%. The absorption with reaction system, in comparison, performed exceedingly well decreasing the CO_2 mole fraction by as much as 17.5 mol-% from 17.8 mol-% at the inlet to under 3 mol-% at the outlet. Both sets of data are meaningful and will be useful in developing the model.

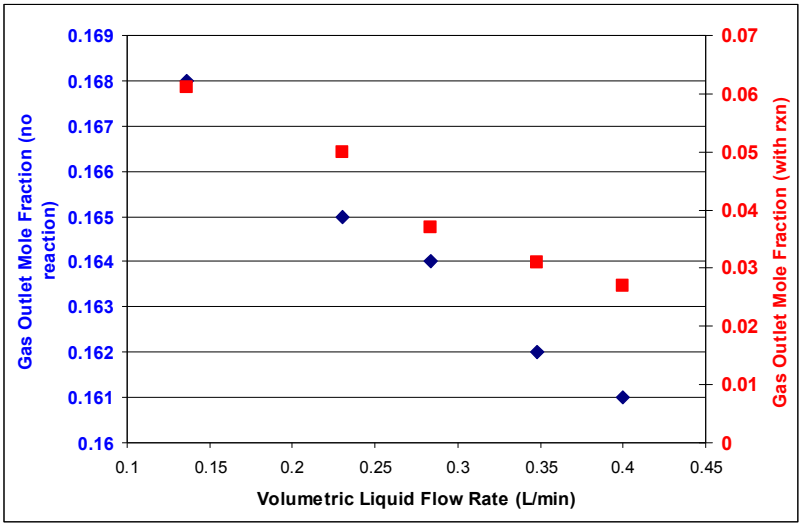

Figure 8: Output concentration versus volumetric liquid flow rate for simple absorption (blue) and absorption with reaction (red).

During both experiments, it was qualitatively determined that heat effects were minimal within the absorption column. This indicated that a detailed energy balance could be neglected from the final teaching aid in order keep it as easy to understand as possible.

4.3 Modeled Absorption/ Reaction System

4.3.1 Overall Mass Transfer Coefficient

After performing the parametric optimization on the overall mass transfer coefficient, $K_y a$, a strong linear correlation was observed between the coefficient and the liquid flow rate.

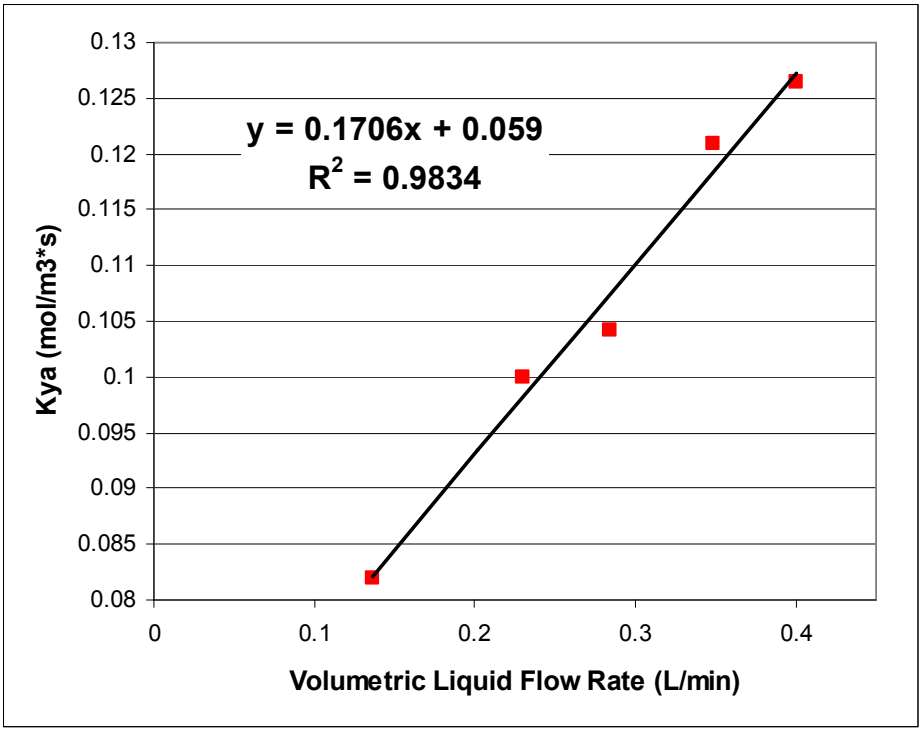

Figure 9: Correlation of overall mass transfer coefficient versus liquid flow rate for simple absorption in miniature column.

By using the equation

$$K_y a = 0.1706 * W + 0.059$$

For the overall mass transfer coefficient instead of merely using a different constant at each water flow rate, the final model is obtained which can be used to explore the miniature absorption column operating at *any* flow rate in the range of approximately 0.1 to 0.4 L/min.

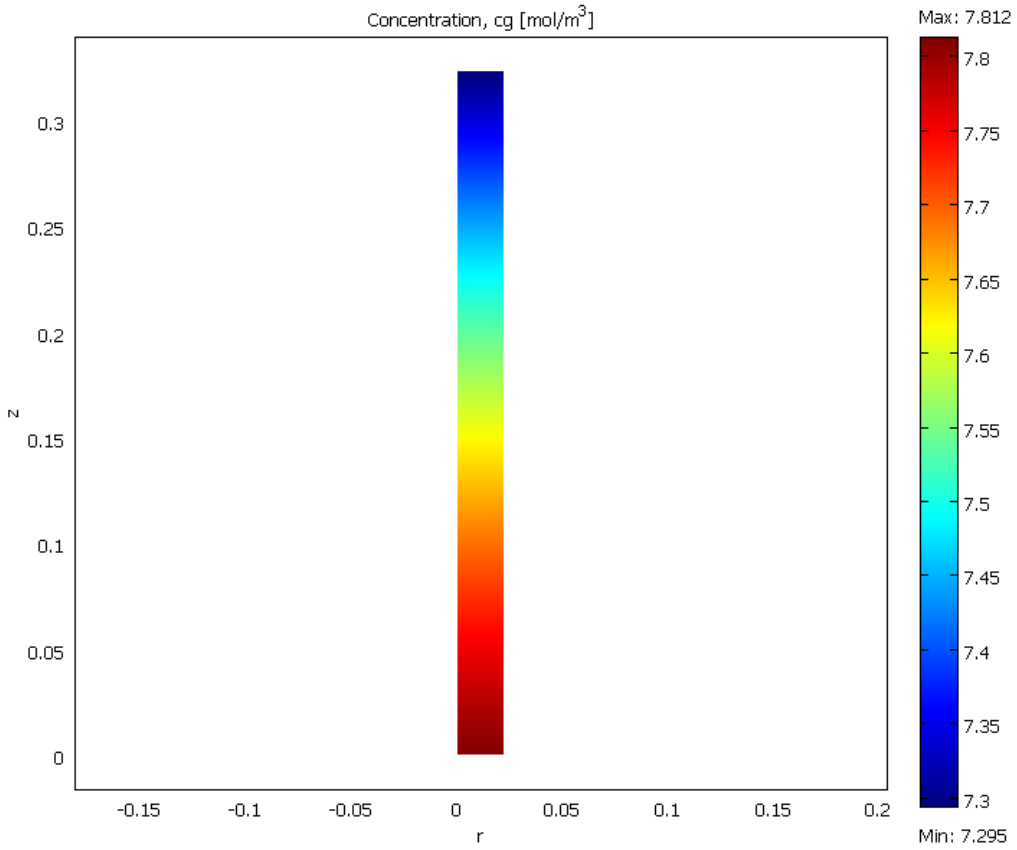

Figure 10: Estimated gas phase concentration profile for column operating at 0.3 L/min liquid flow rate

4.3.2 Gas Phase Mass Transfer Coefficient

Using the above obtained mass transfer coefficient with known kinetics data, it was quickly seen that the overall mass transfer coefficient was not the appropriate way to model the system undergoing reaction.

Table 5: Calculated and Experimental Outlet concentrations for absorption/reaction system.

Liquid Flow (L/min)	Y Out, Experimental	Y Out, Calculated	Y Out, No Rxn
0.23	**0.05**	**0.165**	**0.165**
0.284	**0.037**	**0.163**	**0.164**
0.348	**0.031**	**0.162**	**0.162**
0.4	**0.027**	**0.161**	**0.161**

By using the overall mass transfer coefficient that includes liquid phase mass transfer resistance, almost no CO_2 is able to react within the liquid phase causing the model to predict results nearly identical to the experimental data for the simple absorption system. A better approach is to assume no liquid phase transfer resistance and to use the experimental data to find a second correlation for the overall mass transfer coefficient.

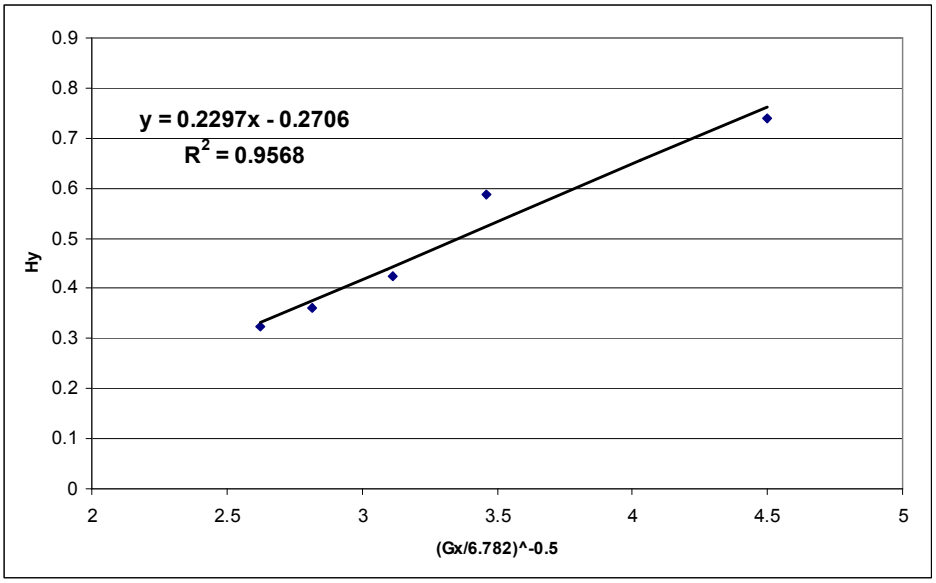

Figure 11: Correlation of gas phase mass transfer coefficient veruss superficial liquid velocity raised to the inverse one half power

Once the gas phase mass transfer coefficient was obtained, it was converted into a gas phase mass transfer resistance, H_y. Similarly, liquid volumetric flow was converted to a superficial velocity, G_x. Plotting these showed a strong linear correlation between H_y and $G_x^{-0.5}$. An equation of this form is in agreement with the empirical correlation provided by Geankoplis. Converting this correlation back to overall mass transfer coefficients and liquid flow rate:

$$k_y a = \frac{1}{0.2812 * W^{-0.5} - 0.2706}$$

Again, this equation can be substituted back into the model in order to use the model at any liquid flow rate between approximately 0.1 to 0.4 L/min.

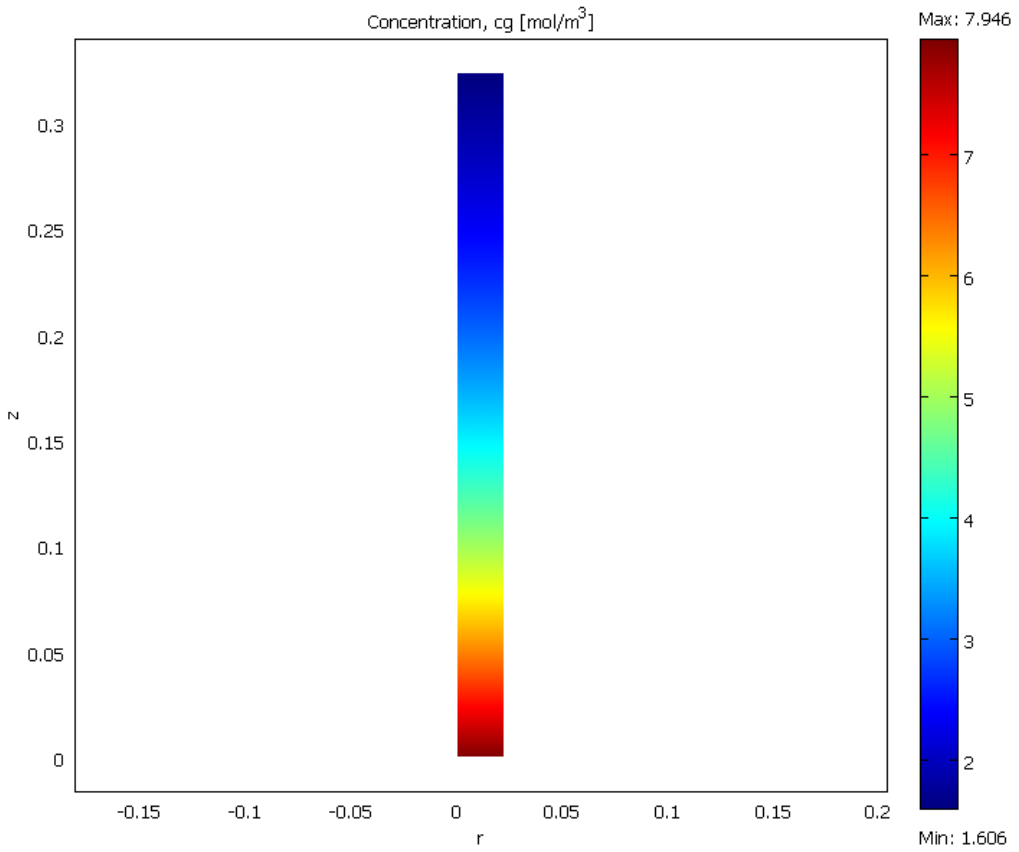

Figure 12: Estimated gas phase concentration profile for column operating at 0.3 L/min liquid flow rate for absorption with reaction system. Note the significant decrease in outlet concentration as compared to the simple absorption model.

4.3.3 Two-Film Absorption with Reaction Model

As stated before, once the overall gas phase mass transfer coefficient is known, it is easy to adjust the parameters in the basic two-film model to accommodate chemical reaction in the liquid phase.

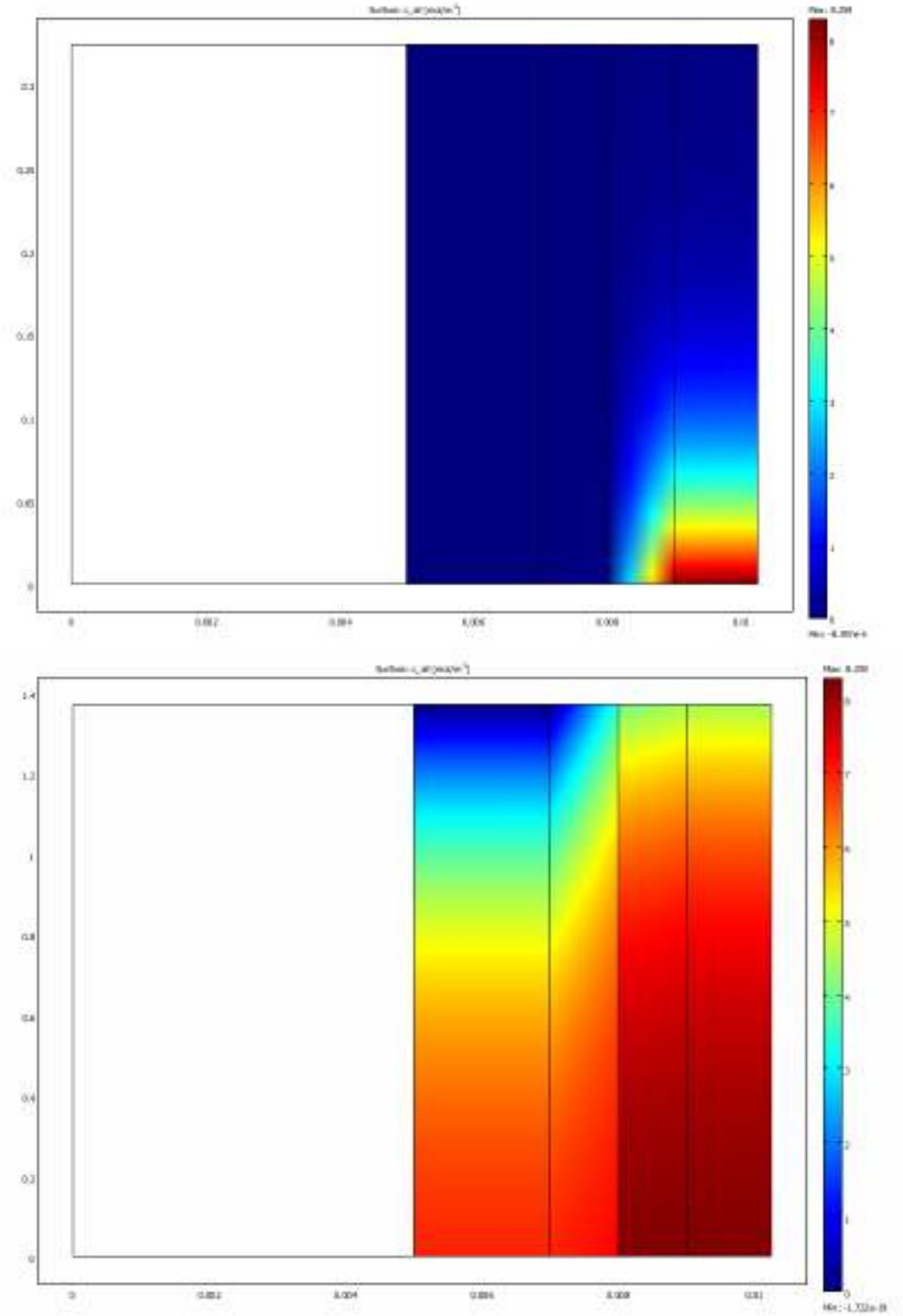

Figure 13: (top) absorption with chemical reaction in miniature column. (Bottom) Simple absorption in pilot scale column.

The resulting model over predicts the amount of CO_2 being removed from the liquid phase. In fact, all of the CO_2 is removed within the column for all flow rates in the range 0.1 to 0.4 L/min. This error could a result of any number of the small experimental errors and theoretical simplifications that have been during the development of this model.

What is important to see is that the drastic differences between this new model and a simple absorption model. When these two models are compared, it is very easy to understand the effects of adding the liquid phase chemical reaction. Predominately, without reaction, the liquid phase is quickly saturated with carbon dioxide. Once chemical reaction is added, practically no dissolved CO_2 is present. It has all been converted into CO_3^{2-}. As a result of this rapid removal from the liquid phase, significantly greater quantities of the CO_2 can be removed from the gas phase.

Therefore, although the new model is not 100% accurate in comparison to experimental data, it simulates the appropriate behavior and will make a useful tool for students trying to explore this advanced form of absorption.

5 Conclusions

After reexamining the pilot scale absorption column, it was determined that heat effects within the system were negligible. The apparent discrepancy with the energy balance was simply a result of thermocouple error. This determination allowed for the models to be simplified by excluding energy balances. Although a full analysis of the system would in fact include an energy balance, this would only add unnecessary complexity to the teaching aid when its purpose is to show the difference of adding a chemical reaction and not the weak temperature effects.

For the actual teaching aid, a decent set of experimental data was collected using a miniature absorption column. This data was then analyzed to determine fitted parameters for the absorption models. The resulting two-film model had a small degree of error, but was sufficiently accurate to successfully demonstrate the advantages of using chemical reaction in combination with absorption. Although the current model is limited to only varying the liquid flow rate, this does not limit the models value. In fact, in industrial settings, the gas stream that must be cleaned of contaminates is typically provided at a fixed rate. Thus the engineering only has access to the liquid flow rate and the column dimensions in order to achieve the desired purification of the gas stream.

In the future, several tasks could be performed to possibly improve the accuracy and flexibility of the model. First, repetition of the experimental results could confirm their accuracy. Then, by changing the gas flow rates, the model could be modified to account for both a variable liquid and gas rate instead of just a variable liquid rate. Finally, it is possible that there is, in fact, a small amount of liquid phase resistance to mass transfer. By adding in this small resistance, it is possible that the appropriate output compositions would be achieved for the system. Additional experiments and literature review would be necessary to investigate this possibility.

6 References

Clark, W. M. "COMSOL Multiphysics Models for Teaching Chemical Engineering Fundamentals: Absorption Column Models and Illustration of the Two-Film Theory of Mass Transfer." 2008.

Geankoplis. *Transport Processes and Separation Process Principles*. Prentice Hall: Upper Saddle River, NJ, 2003

Incropera, Dewitt, Bergman, and Lavine. *Introduction to Heat Transfer*. 5th ed. John Wiley & Sons: USA, 2007.

M Taghizadeh et al. *Chemical Engineering Journal* **82** (2001) 143-148.

7 Appendix 1: Sodium Hydroxide MSDS[8]

MSDS Number: **S4034** * * * * * *Effective Date:* ***05/04/07*** * * * * * *Supercedes:* ***07/07/04***

MSDS Material Safety Data Sheet

From: Mallinckrodt Baker, Inc.
222 Red School Lane
Phillipsburg, NJ 08865

Mallinckrodt CHEMICALS | J.T.Baker

24 Hour Emergency Telephone: 908-859-2151
CHEMTREC: 1-800-424-9300

National Response in Canada
CANUTEC: 613-996-6666

Outside U.S. and Canada
Chemtrec: 703-527-3887

NOTE: CHEMTREC, CANUTEC and National Response Center emergency numbers to be used only in the event of chemical emergencies involving a spill, leak, fire, exposure or accident involving chemicals.

All non-emergency questions should be directed to Customer Service (1-800-582-2537) for assistance.

SODIUM HYDROXIDE

1. Product Identification
Synonyms: Caustic soda; lye; sodium hydroxide solid; sodium hydrate
CAS No.: 1310-73-2
Molecular Weight: 40.00
Chemical Formula: NaOH
Product Codes:
J.T. Baker: 1508, 3717, 3718, 3721, 3722, 3723, 3728, 3734, 3736, 5045, 5565
Mallinckrodt: 7001, 7680, 7708, 7712, 7772, 7798

2. Composition/Information on Ingredients

Ingredient	CAS No	Percent	Hazardous
Sodium Hydroxide	1310-73-2	99 - 100%	Yes

3. Hazards Identification
Emergency Overview

POISON! DANGER! CORROSIVE. MAY BE FATAL IF SWALLOWED. HARMFUL IF INHALED. CAUSES BURNS TO ANY AREA OF CONTACT.

[8] http://www.jtbaker.com/msds/englishhtml/s4034.htm

REACTS WITH WATER, ACIDS AND OTHER MATERIALS.

SAF-T-DATA(tm) Ratings (Provided here for your convenience)

Health Rating: 4 - Extreme (Poison)
Flammability Rating: 0 - None
Reactivity Rating: 2 - Moderate
Contact Rating: 4 - Extreme (Corrosive)
Lab Protective Equip: GOGGLES & SHIELD; LAB COAT & APRON; VENT HOOD; PROPER GLOVES
Storage Color Code: White Stripe (Store Separately)

Potential Health Effects

Inhalation:
Severe irritant. Effects from inhalation of dust or mist vary from mild irritation to serious damage of the upper respiratory tract, depending on severity of exposure. Symptoms may include sneezing, sore throat or runny nose. Severe pneumonitis may occur.
Ingestion:
Corrosive! Swallowing may cause severe burns of mouth, throat, and stomach. Severe scarring of tissue and death may result. Symptoms may include bleeding, vomiting, diarrhea, fall in blood pressure. Damage may appear days after exposure.
Skin Contact:
Corrosive! Contact with skin can cause irritation or severe burns and scarring with greater exposures.
Eye Contact:
Corrosive! Causes irritation of eyes, and with greater exposures it can cause burns that may result in permanent impairment of vision, even blindness.
Chronic Exposure:
Prolonged contact with dilute solutions or dust has a destructive effect upon tissue.
Aggravation of Pre-existing Conditions:
Persons with pre-existing skin disorders or eye problems or impaired respiratory function may be more susceptible to the effects of the substance.

---

4. First Aid Measures
Inhalation:
Remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Call a physician.
Ingestion:
DO NOT INDUCE VOMITING! Give large quantities of water or milk if available. Never give anything by mouth to an unconscious person. Get medical attention immediately.
Skin Contact:
Immediately flush skin with plenty of water for at least 15 minutes while removing

contaminated clothing and shoes. Call a physician, immediately. Wash clothing before reuse.

Eye Contact:

Immediately flush eyes with plenty of water for at least 15 minutes, lifting lower and upper eyelids occasionally. Get medical attention immediately.

Note to Physician:

Perform endoscopy in all cases of suspected sodium hydroxide ingestion. In cases of severe esophageal corrosion, the use of therapeutic doses of steroids should be considered. General supportive measures with continual monitoring of gas exchange, acid-base balance, electrolytes, and fluid intake are also required.

---

5. Fire Fighting Measures

Fire:

Not considered to be a fire hazard. Hot or molten material can react violently with water. Can react with certain metals, such as aluminum, to generate flammable hydrogen gas.

Explosion:

Not considered to be an explosion hazard.

Fire Extinguishing Media:

Use any means suitable for extinguishing surrounding fire. Adding water to caustic solution generates large amounts of heat.

Special Information:

In the event of a fire, wear full protective clothing and NIOSH-approved self-contained breathing apparatus with full facepiece operated in the pressure demand or other positive pressure mode.

---

6. Accidental Release Measures

Ventilate area of leak or spill. Keep unnecessary and unprotected people away from area of spill. Wear appropriate personal protective equipment as specified in Section 8. Spills: Pick up and place in a suitable container for reclamation or disposal, using a method that does not generate dust. Do not flush caustic residues to the sewer. Residues from spills can be diluted with water, neutralized with dilute acid such as acetic, hydrochloric or sulfuric. Absorb neutralized caustic residue on clay, vermiculite or other inert substance and package in a suitable container for disposal.

US Regulations (CERCLA) require reporting spills and releases to soil, water and air in excess of reportable quantities. The toll free number for the US Coast Guard National Response Center is (800) 424-8802.

---

7. Handling and Storage

Keep in a tightly closed container. Protect from physical damage. Store in a cool, dry, ventilated area away from sources of heat, moisture and incompatibilities. Always add the caustic to water while stirring; never the reverse. Containers of this material may be hazardous when empty since they retain product residues (dust, solids); observe all warnings and precautions listed for the product. Do not store with aluminum or magnesium. Do not mix with acids or organic materials.

8. Exposure Controls/Personal Protection

Airborne Exposure Limits:

- OSHA Permissible Exposure Limit (PEL):
2 mg/m3 Ceiling
- ACGIH Threshold Limit Value (TLV):
2 mg/m3 Ceiling

Ventilation System:

A system of local and/or general exhaust is recommended to keep employee exposures below the Airborne Exposure Limits. Local exhaust ventilation is generally preferred because it can control the emissions of the contaminant at its source, preventing dispersion of it into the general work area. Please refer to the ACGIH document, *Industrial Ventilation, A Manual of Recommended Practices*, most recent edition, for details.

Personal Respirators (NIOSH Approved):

If the exposure limit is exceeded and engineering controls are not feasible, a half facepiece particulate respirator (NIOSH type N95 or better filters) may be worn for up to ten times the exposure limit or the maximum use concentration specified by the appropriate regulatory agency or respirator supplier, whichever is lowest.. A full-face piece particulate respirator (NIOSH type N100 filters) may be worn up to 50 times the exposure limit, or the maximum use concentration specified by the appropriate regulatory agency, or respirator supplier, whichever is lowest. If oil particles (e.g. lubricants, cutting fluids, glycerine, etc.) are present, use a NIOSH type R or P filter. For emergencies or instances where the exposure levels are not known, use a full-facepiece positive-pressure, air-supplied respirator. WARNING: Air-purifying respirators do not protect workers in oxygen-deficient atmospheres.

Skin Protection:

Wear impervious protective clothing, including boots, gloves, lab coat, apron or coveralls, as appropriate, to prevent skin contact.

Eye Protection:

Use chemical safety goggles and/or a full face shield where splashing is possible. Maintain eye wash fountain and quick-drench facilities in work area.

---

9. Physical and Chemical Properties

Appearance:

White, deliquescent pellets or flakes.

Odor:

Odorless.

Solubility:

111 g/100 g of water.

Specific Gravity:

2.13

pH:

13 - 14 (0.5% soln.)

% Volatiles by volume @ 21C (70F):

0

Boiling Point:
1390C (2534F)
Melting Point:
318C (604F)
Vapor Density (Air=1):
> 1.0
Vapor Pressure (mm Hg):
Negligible.
Evaporation Rate (BuAc=1):
No information found.

---

10. Stability and Reactivity
Stability:
Stable under ordinary conditions of use and storage. Very hygroscopic. Can slowly pick up moisture from air and react with carbon dioxide from air to form sodium carbonate.
Hazardous Decomposition Products:
Sodium oxide. Decomposition by reaction with certain metals releases flammable and explosive hydrogen gas.
Hazardous Polymerization:
Will not occur.
Incompatibilities:
Sodium hydroxide in contact with acids and organic halogen compounds, especially trichloroethylene, may causes violent reactions. Contact with nitromethane and other similar nitro compounds causes formation of shock-sensitive salts. Contact with metals such as aluminum, magnesium, tin, and zinc cause formation of flammable hydrogen gas. Sodium hydroxide, even in fairly dilute solution, reacts readily with various sugars to produce carbon monoxide. Precautions should be taken including monitoring the tank atmosphere for carbon monoxide to ensure safety of personnel before vessel entry.
Conditions to Avoid:
Moisture, dusting and incompatibles.

---

11. Toxicological Information

Irritation data: skin, rabbit: 500 mg/24H severe; eye rabbit: 50 ug/24H severe; investigated as a mutagen.

--------\Cancer Lists\----------

Ingredient	---NTP Carcinogen--- Known	Anticipated	IARC Category
Sodium Hydroxide (1310-73-2)	No	No	None

---

12. Ecological Information
Environmental Fate:
No information found.

Environmental Toxicity:
No information found.

---

13. Disposal Considerations
Whatever cannot be saved for recovery or recycling should be handled as hazardous waste and sent to a RCRA approved waste facility. Processing, use or contamination of this product may change the waste management options. State and local disposal regulations may differ from federal disposal regulations. Dispose of container and unused contents in accordance with federal, state and local requirements.

---

14. Transport Information
Domestic (Land, D.O.T.)

Proper Shipping Name: SODIUM HYDROXIDE, SOLID
Hazard Class: 8
UN/NA: UN1823
Packing Group: II
Information reported for product/size: 300LB

International (Water, I.M.O.)

Proper Shipping Name: SODIUM HYDROXIDE, SOLID
Hazard Class: 8
UN/NA: UN1823
Packing Group: II
Information reported for product/size: 300LB

---

15. Regulatory Information

--------\Chemical Inventory Status - Part 1\--------

Ingredient	TSCA	EC	Japan	Australia
Sodium Hydroxide (1310-73-2)	Yes	Yes	Yes	Yes

--------\Chemical Inventory Status - Part 2\--------

		--Canada--		
Ingredient	Korea	DSL	NDSL	Phil.
Sodium Hydroxide (1310-73-2)	Yes	Yes	No	Yes

--------\Federal, State & International Regulations - Part 1\--------

Ingredient	-SARA 302- RQ	TPQ	List	------SARA 313------ Chemical Catg.
Sodium Hydroxide (1310-73-2)	No	No	No	No

--------\Federal, State & International Regulations - Part 2\--------

Ingredient	CERCLA	-RCRA- 261.33	- TSCA- 8(d)
Sodium Hydroxide (1310-73-2)	1000	No	No

Chemical Weapons Convention: No TSCA 12(b): No CDTA: No
SARA 311/312: Acute: Yes Chronic: No Fire: No Pressure: No
Reactivity: Yes (Pure / Solid)

Australian Hazchem Code: 2R
Poison Schedule: S6
WHMIS:
This MSDS has been prepared according to the hazard criteria of the Controlled Products Regulations (CPR) and the MSDS contains all of the information required by the CPR.

---

16. Other Information
NFPA Ratings: Health: **3** Flammability: **0** Reactivity: **1**
Label Hazard Warning:
POISON! DANGER! CORROSIVE. MAY BE FATAL IF SWALLOWED. HARMFUL IF INHALED. CAUSES BURNS TO ANY AREA OF CONTACT. REACTS WITH WATER, ACIDS AND OTHER MATERIALS.
Label Precautions:
Do not get in eyes, on skin, or on clothing.
Do not breathe dust.
Keep container closed.
Use only with adequate ventilation.
Wash thoroughly after handling.
Label First Aid:
If swallowed, DO NOT INDUCE VOMITING. Give large quantities of water. Never give anything by mouth to an unconscious person. In case of contact, immediately flush eyes or skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen. In all cases get medical attention immediately.
Product Use:

Laboratory Reagent.

Revision Information:

No Changes.

Disclaimer:

****

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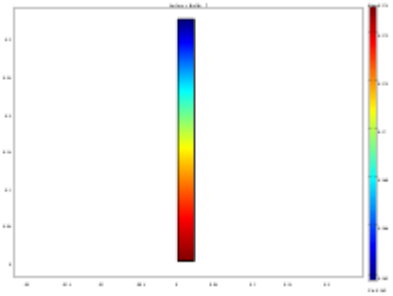
Prepared by: Environmental Health & Safety
Phone Number: (314) 654-1600 (U.S.A.)

8 Appendix 2: Mini-Absorber, Lumped Parameter Model for Simple Absorption

COMSOL Model Report



1. Table of Contents

2. Model Properties

Property	**Value**
Model name	
Author	
Company	
Department	
Reference	
URL	
Saved date	Apr 15, 2009 4:39:48 PM
Creation date	Jun 11, 2008 1:16:28 PM
COMSOL version	COMSOL 3.5.0.603

File name: R:\Absorption\absorber-mini.mph

Application modes and modules used in this model:

- Geom1 (Axial symmetry (2D))

- Convection and Diffusion (Chemical Engineering Module)
- Convection and Diffusion (Chemical Engineering Module)

3. Constants

Name	Expression	Value	Description
W	.284		water rate in (L/min)
A	1.5		air rate in (L/min)
yin	.175		mole fraction CO2 in
Kh	614.26*W+212.25		mass trans coeff (mol/m3h)
H	1420		Henrys constant (atm)
K	Kh/3600		mass trans coeff (mol/m3s)
vl	-(W*1000/100^3/60/4.56e-3)		liquid velocity (m/s)
vgo	A*1000/100^3/60/4.56e-3		air velocity in (m/s)
cl0	0		liquid CO2 conc. in (mol/m3)
cg0	yin*101325/8.314/273		gas CO2 conc. in (mol/m3)
Dg	1.6e-5		diff. coeff. gas (m2/s)
Dl	1.8e-9		diff. coeff. liquid (m2./s)

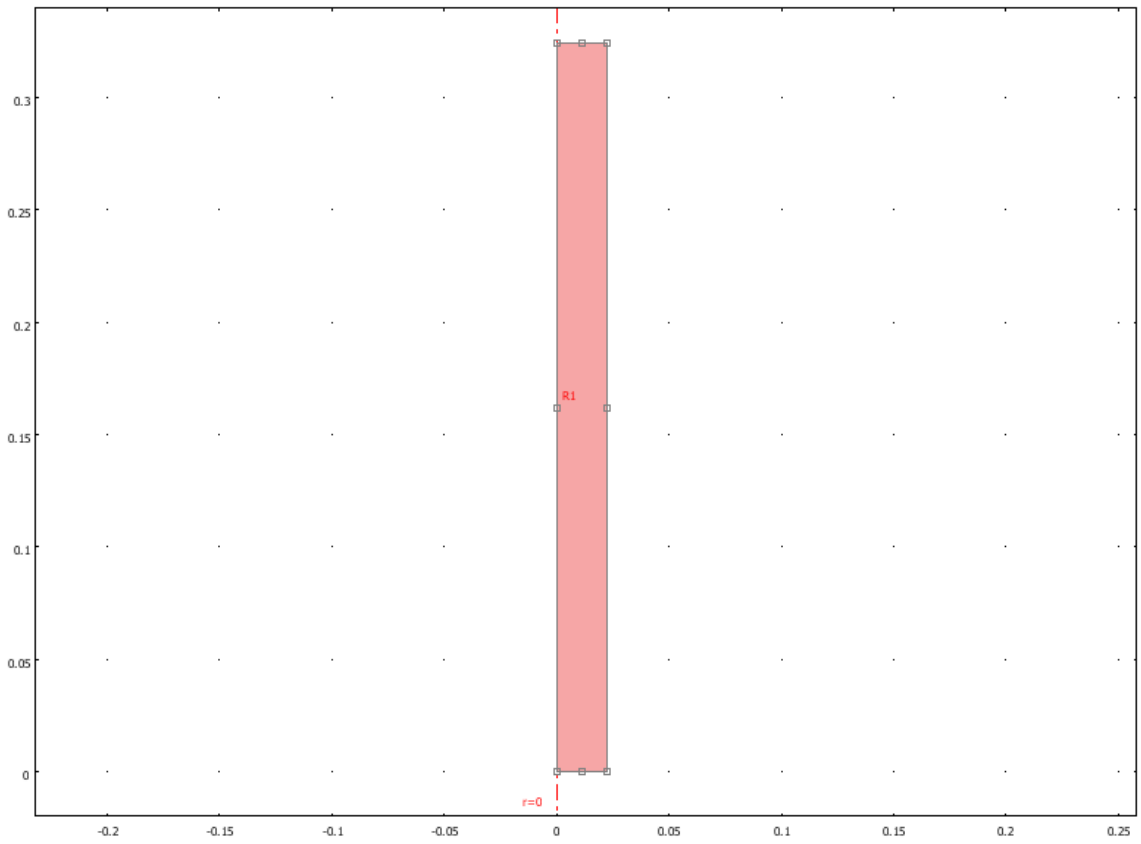
4. Global Expressions

Name	Expression	Unit	Description
y	cg*8.314*273/101325	mol/m^3	
x	cl*1000/55.55/100^3	mol/m^3	
ye	H*x	mol/m^3	
vg	vgo/(1-y)	m^3/mol	

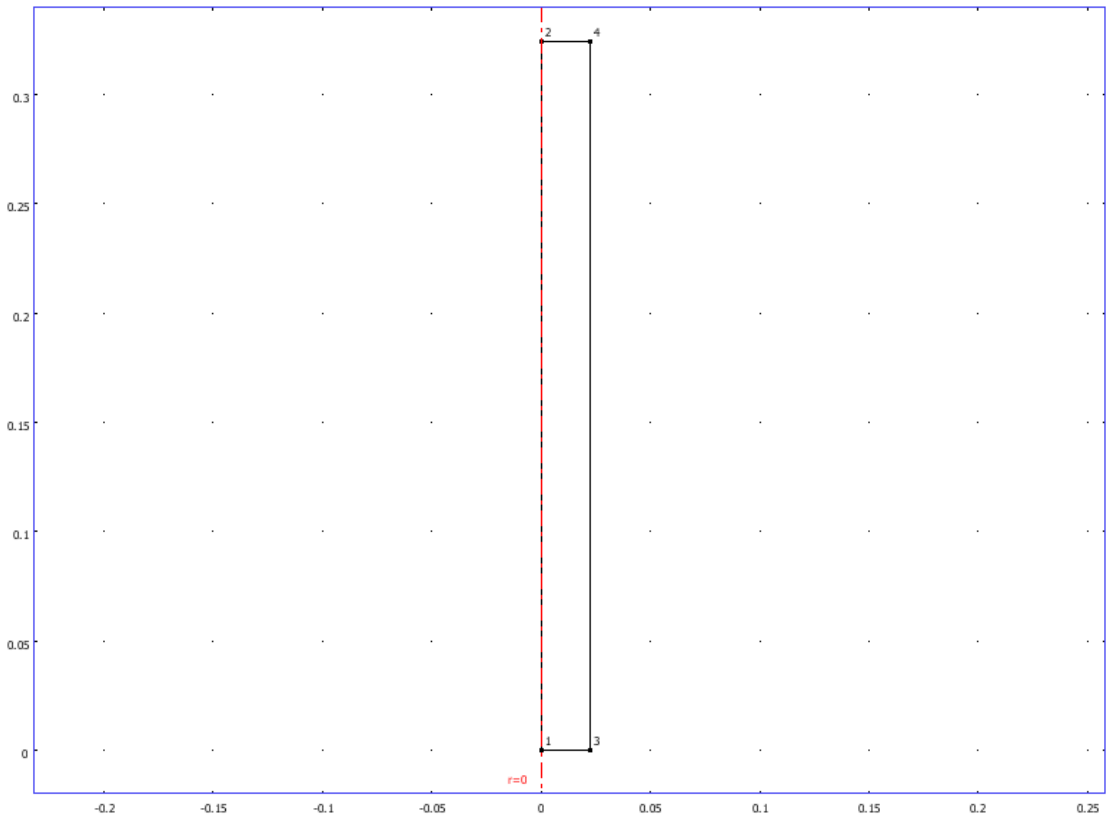
5. Geometry

Number of geometries: 1

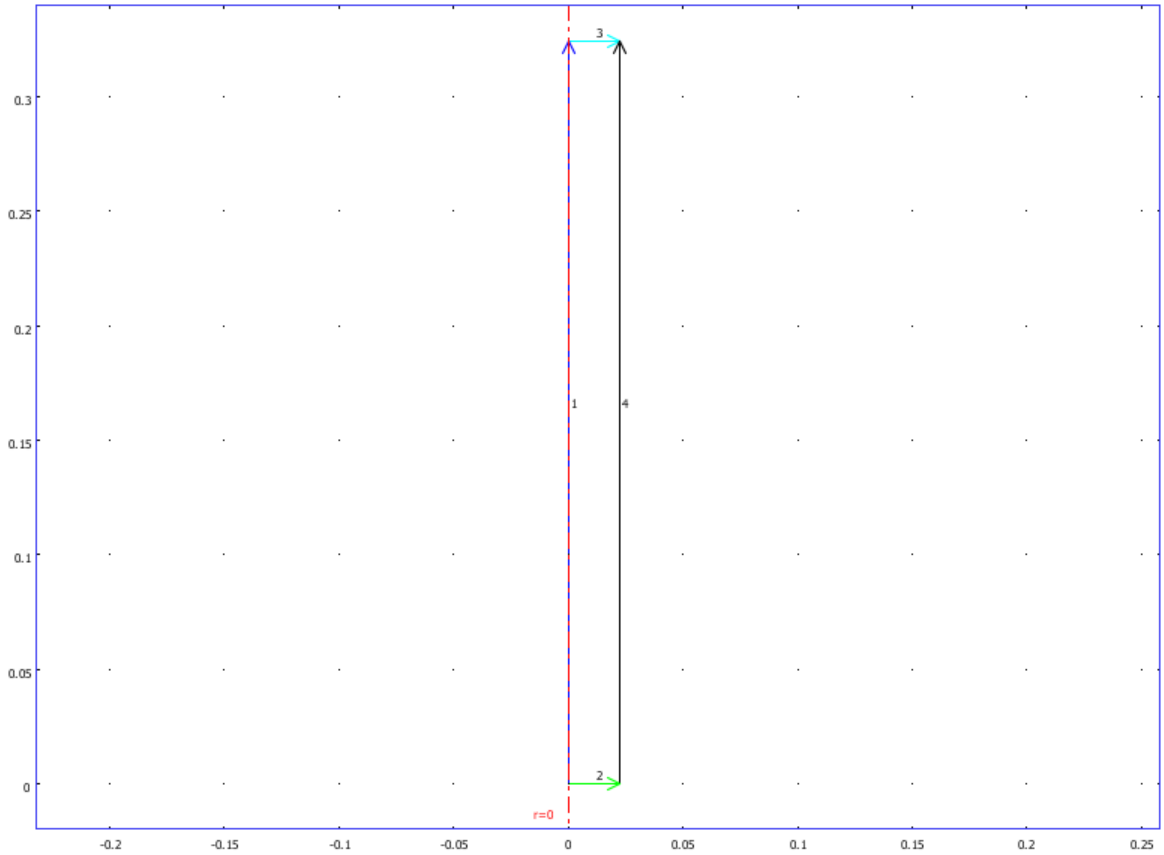
5.1. Geom1



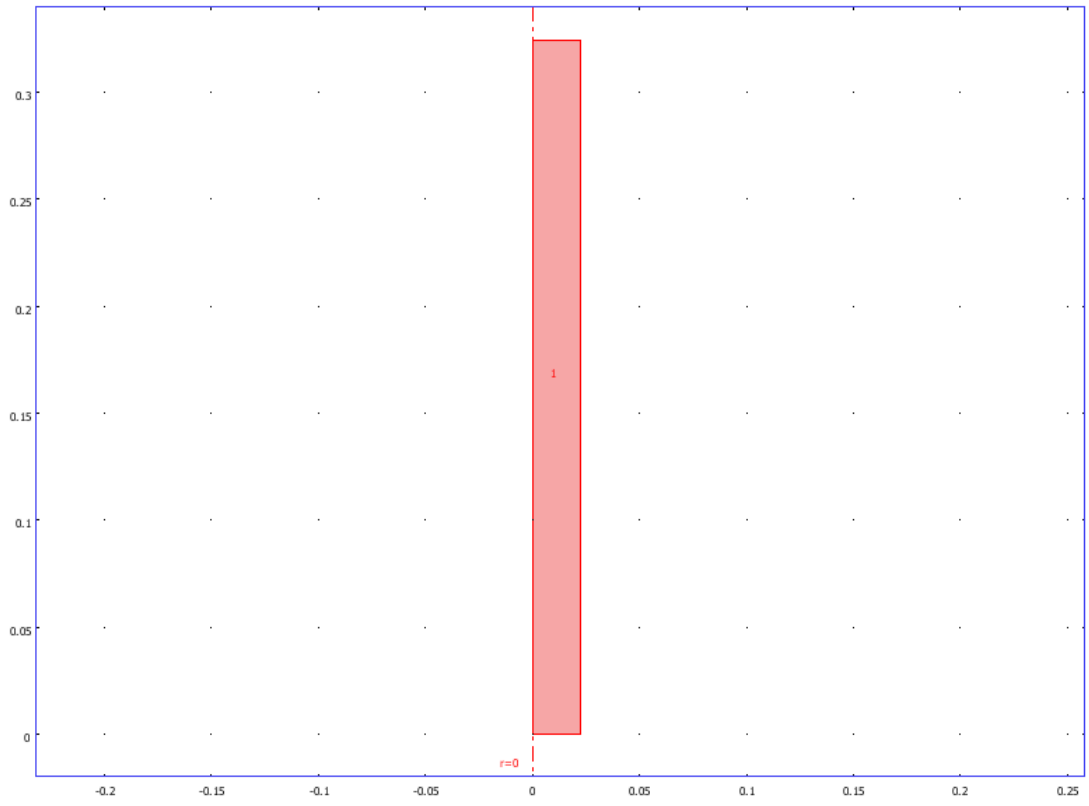
5.1.1. Point mode



5.1.2. Boundary mode



5.1.3. Subdomain mode



6. Geom1

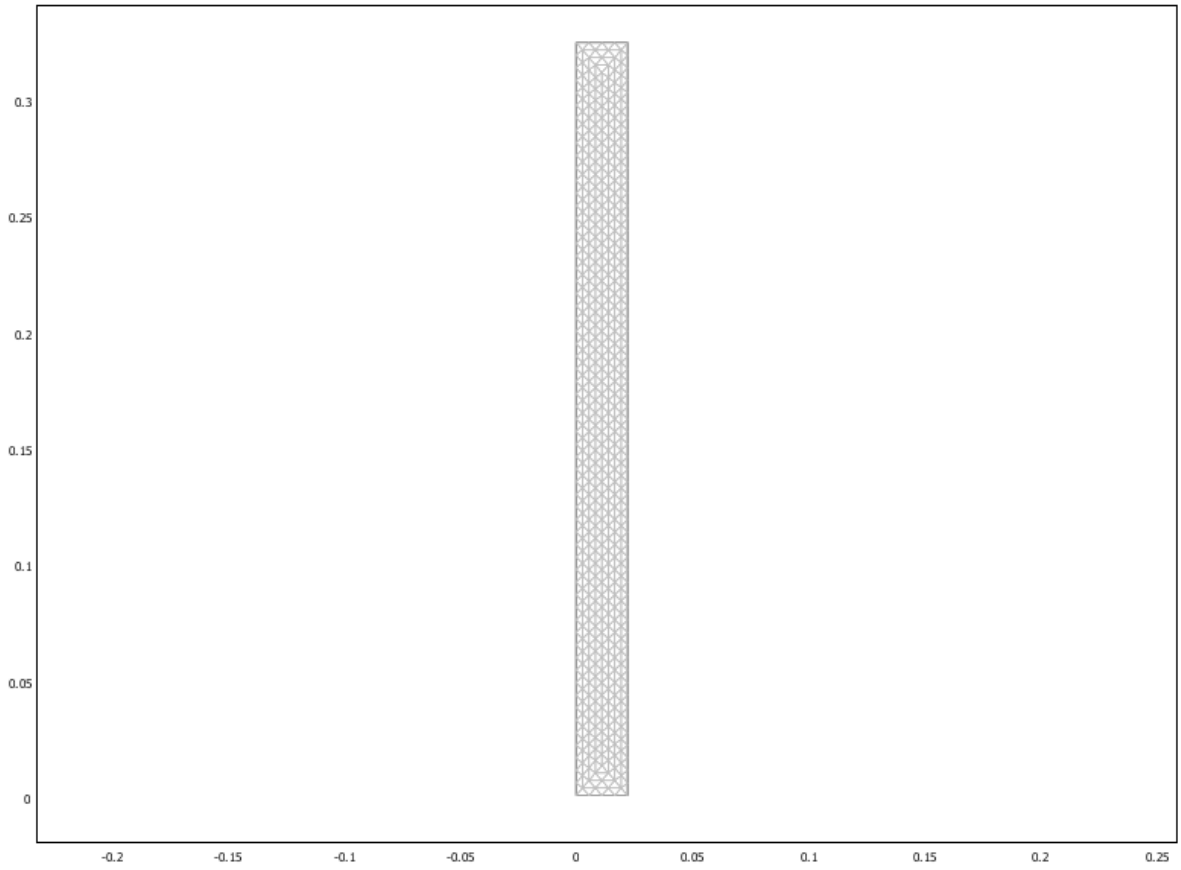
Space dimensions: Axial symmetry (2D)

Independent variables: r, phi, z

6.1. Mesh

6.1.1. Mesh Statistics

Number of degrees of freedom	4098
Number of mesh points	545
Number of elements	960
Triangular	960
Quadrilateral	0
Number of boundary elements	128
Number of vertex elements	4
Minimum element quality	0.87
Element area ratio	0.75



6.2. Application Mode: Convection and Diffusion (chcd)

Application mode type: Convection and Diffusion (Chemical Engineering Module)

Application mode name: chcd

6.2.1. Application Mode Properties

Property	**Value**
Default element type	Lagrange - Quadratic
Analysis type	Stationary
Equation form	Non-conservative
Equilibrium assumption	Off
Frame	Frame (ref)
Weak constraints	Off
Constraint type	Ideal

6.2.2. Variables

Dependent variables: cg

Shape functions: shlag(2,'cg')

Interior boundaries not active

6.2.3. Boundary Settings

Boundary		1	2	3
Type		Axial symmetry	Concentration	Convective flux
Concentration (c0)	mol/m^3	0	**cg0**	0

Boundary		4
Type		Insulation/Symmetry
Concentration (c0)	mol/m^3	0

6.2.4. Subdomain Settings

Subdomain		1
Diffusion coefficient (D)	m^2/s	**Dg**
Reaction rate (R)	$mol/(m^3 \cdot s)$	**-K*(1-y)*(y-ye)**
z-velocity (v)	m/s	**vg**

6.3. Application Mode: Convection and Diffusion (chcd2)

Application mode type: Convection and Diffusion (Chemical Engineering Module)

Application mode name: chcd2

6.3.1. Application Mode Properties

Property	**Value**
Default element type	Lagrange - Quadratic
Analysis type	Stationary
Equation form	Non-conservative
Equilibrium assumption	Off
Frame	Frame (ref)
Weak constraints	Off
Constraint type	Ideal

6.3.2. Variables

Dependent variables: cl

Shape functions: shlag(2,'cl')

Interior boundaries not active

6.3.3. Boundary Settings

Boundary		1	2	3
Type		Axial symmetry	Convective flux	Concentration
Concentration (c0)	mol/m^3	0	0	**cl0**

Boundary		4
Type		Insulation/Symmetry
Concentration (c0)	mol/m^3	0

6.3.4. Subdomain Settings

Subdomain		1
Diffusion coefficient (D)	m^2/s	**Dl**
Reaction rate (R)	$mol/(m^3 \cdot s)$	**K*(y-ye)**
z-velocity (v)	m/s	**vl**

7. Solver Settings

Solve using a script: off

Analysis type	Stationary
Auto select solver	On
Solver	Stationary
Solution form	Automatic
Symmetric	auto
Adaptive mesh refinement	Off
Optimization/Sensitivity	Off
Plot while solving	Off

7.1. Direct (UMFPACK)

Solver type: Linear system solver

Parameter	**Value**
Pivot threshold	0.1
Memory allocation factor	0.7

7.2. Stationary

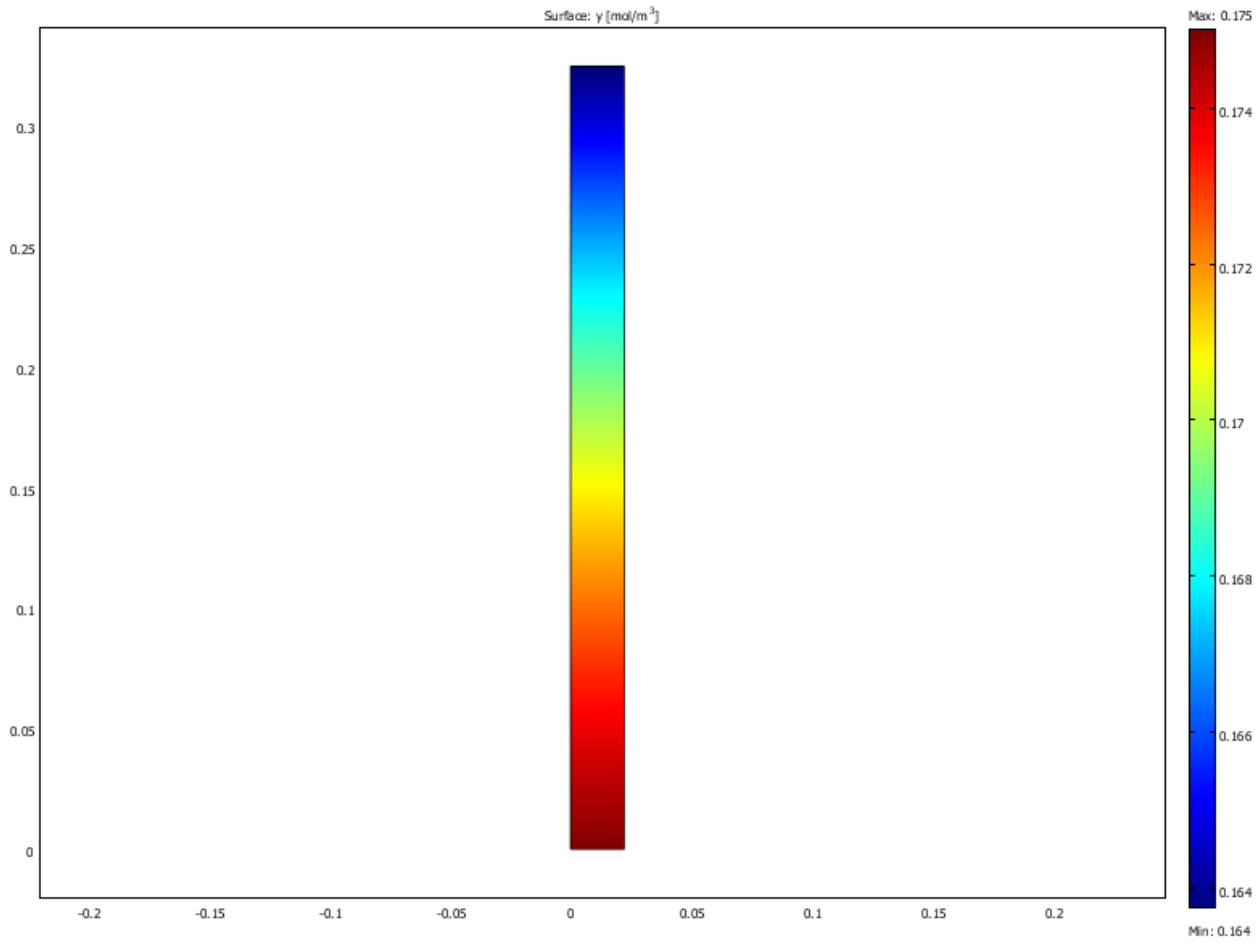
Parameter	**Value**
Linearity	Automatic
Relative tolerance	1.0E-6
Maximum number of iterations	25
Manual tuning of damping parameters	Off

Highly nonlinear problem	Off
Initial damping factor	1.0
Minimum damping factor	1.0E-4
Restriction for step size update	10.0

7.3. Advanced

Parameter	**Value**
Constraint handling method	Elimination
Null-space function	Automatic
Automatic assembly block size	On
Assembly block size	5000
Use Hermitian transpose of constraint matrix and in symmetry detection	Off
Use complex functions with real input	Off
Stop if error due to undefined operation	On
Store solution on file	Off
Type of scaling	Automatic
Manual scaling	
Row equilibration	On
Manual control of reassembly	Off
Load constant	On
Constraint constant	On
Mass constant	On
Damping (mass) constant	On
Jacobian constant	On
Constraint Jacobian constant	On

8. Postprocessing



9. Variables

9.1. Boundary

Name	Description	Unit	Expression
ndflux_cg_chcd	Normal diffusive flux, cg	mol/(m^2*s)	nr_chcd * dflux_cg_r_chcd+nz_chcd * dflux_cg_z_chcd
ncflux_cg_chcd	Normal convective flux, cg	mol/(m^2*s)	nr_chcd * cflux_cg_r_chcd+nz_chcd * cflux_cg_z_chcd
ntflux_cg_chcd	Normal total flux, cg	mol/(m^2*s)	nr_chcd * tflux_cg_r_chcd+nz_chcd * tflux_cg_z_chcd
ndflux_cl_chcd2	Normal diffusive flux, cl	mol/(m^2*s)	nr_chcd2 * dflux_cl_r_chcd2+nz_chcd2 * dflux_cl_z_chcd2
ncflux_cl_chcd2	Normal convective flux, cl	mol/(m^2*s)	nr_chcd2 * cflux_cl_r_chcd2+nz_chcd2 * cflux_cl_z_chcd2
ntflux_cl_chcd2	Normal total flux, cl	mol/(m^2*s)	nr_chcd2 * tflux_cl_r_chcd2+nz_chcd2 * tflux_cl_z_chcd2

9.2. Subdomain

Name	Description	Unit	Expression
grad_cg_r_chcd	Concentration gradient, cg, r component	mol/m^4	cgr
dflux_cg_r_chcd	Diffusive flux, cg, r component	mol/(m^2*s)	-Drr_cg_chcd * cgr-Drz_cg_chcd * cgz
cflux_cg_r_chcd	Convective flux, cg, r component	mol/(m^2*s)	cg * u_cg_chcd
tflux_cg_r_chcd	Total flux, cg, r component	mol/(m^2*s)	dflux_cg_r_chcd+cflux_cg_r_chcd
grad_cg_z_chcd	Concentration gradient, cg, z component	mol/m^4	cgz
dflux_cg_z_chcd	Diffusive flux, cg, z component	mol/(m^2*s)	-Dzr_cg_chcd * cgr-Dzz_cg_chcd * cgz
cflux_cg_z_chcd	Convective flux, cg, z component	mol/(m^2*s)	cg * v_cg_chcd
tflux_cg_z_chcd	Total flux, cg, z component	mol/(m^2*s)	dflux_cg_z_chcd+cflux_cg_z_chcd
beta_cg_r_chcd	Convective field, cg, r component	m^2/s	r * u_cg_chcd
beta_cg_z_chcd	Convective field, cg, z component	m^2/s	r * v_cg_chcd
grad_cg_chcd	Concentration gradient, cg	mol/m^4	sqrt(grad_cg_r_chcd^2+grad_cg_z_chcd^2)
dflux_cg_chcd	Diffusive flux, cg	mol/(m^2*s)	sqrt(dflux_cg_r_chcd^2+dflux_cg_z_chcd^2)

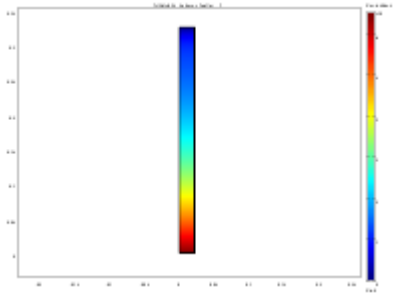
cflux_cg_chcd	Convective flux, cg	mol/(m^2*s)	sqrt(cflux_cg_r_chcd^2+cflux_cg_z_chcd^2)
tflux_cg_chcd	Total flux, cg	mol/(m^2*s)	sqrt(tflux_cg_r_chcd^2+tflux_cg_z_chcd^2)
cellPe_cg_chcd	Cell Peclet number, cg	1	h * sqrt(beta_cg_r_chcd^2+beta_cg_z_chcd^2)/Dm_cg_chcd
Dm_cg_chcd	Mean diffusion coefficient, cg	m^3/s	r * (Drr_cg_chcd * u_cg_chcd^2+Drz_cg_chcd * u_cg_chcd * v_cg_chcd+Dzr_cg_chcd * v_cg_chcd * u_cg_chcd+Dzz_cg_chcd * v_cg_chcd^2)/(u_cg_chcd^2+v_cg_chcd^2+eps)
res_cg_chcd	Equation residual for cg	mol/(m^2*s)	r * (-Drr_cg_chcd * cgrr-Drz_cg_chcd * cgrz+cgr * u_cg_chcd-Dzr_cg_chcd * cgzr-Dzz_cg_chcd * cgzz+cgz * v_cg_chcd-R_cg_chcd)
res_sc_cg_chcd	Shock capturing residual for cg	mol/(m^2*s)	r * (cgr * u_cg_chcd+cgz * v_cg_chcd-R_cg_chcd)
da_cg_chcd	Total time scale factor, cg	m	r * Dts_cg_chcd
grad_cl_r_chcd2	Concentration gradient, cl, r component	mol/m^4	clr
dflux_cl_r_chcd2	Diffusive flux, cl, r component	mol/(m^2*s)	-Drr_cl_chcd2 * clr-Drz_cl_chcd2 * clz
cflux_cl_r_chcd2	Convective flux, cl, r component	mol/(m^2*s)	cl * u_cl_chcd2
tflux_cl_r_chcd2	Total flux, cl, r component	mol/(m^2*s)	dflux_cl_r_chcd2+cflux_cl_r_chcd2
grad_cl_z_chcd2	Concentration gradient, cl, z component	mol/m^4	clz
dflux_cl_z_ch	Diffusive	mol/(m^2	-Dzr_cl_chcd2 * clr-Dzz_cl_chcd2 * clz

cd2	flux, cl, z component	*s)	
cflux_cl_z_chcd2	Convective flux, cl, z component	mol/(m^2*s)	cl * v_cl_chcd2
tflux_cl_z_chcd2	Total flux, cl, z component	mol/(m^2*s)	dflux_cl_z_chcd2+cflux_cl_z_chcd2
beta_cl_r_chcd2	Convective field, cl, r component	m^2/s	r * u_cl_chcd2
beta_cl_z_chcd2	Convective field, cl, z component	m^2/s	r * v_cl_chcd2
grad_cl_chcd2	Concentration gradient, cl	mol/m^4	sqrt(grad_cl_r_chcd2^2+grad_cl_z_chcd2^2)
dflux_cl_chcd2	Diffusive flux, cl	mol/(m^2*s)	sqrt(dflux_cl_r_chcd2^2+dflux_cl_z_chcd2^2)
cflux_cl_chcd2	Convective flux, cl	mol/(m^2*s)	sqrt(cflux_cl_r_chcd2^2+cflux_cl_z_chcd2^2)
tflux_cl_chcd2	Total flux, cl	mol/(m^2*s)	sqrt(tflux_cl_r_chcd2^2+tflux_cl_z_chcd2^2)
cellPe_cl_chcd2	Cell Peclet number, cl	1	h * sqrt(beta_cl_r_chcd2^2+beta_cl_z_chcd2^2)/Dm_cl_chcd2
Dm_cl_chcd2	Mean diffusion coefficient, cl	m^3/s	r * (Drr_cl_chcd2 * u_cl_chcd2^2+Drz_cl_chcd2 * u_cl_chcd2 * v_cl_chcd2+Dzr_cl_chcd2 * v_cl_chcd2 * u_cl_chcd2+Dzz_cl_chcd2 * v_cl_chcd2^2)/(u_cl_chcd2^2+v_cl_chcd2^2+eps)
res_cl_chcd2	Equation residual for cl	mol/(m^2*s)	r * (-Drr_cl_chcd2 * clrr-Drz_cl_chcd2 * clrz+clr * u_cl_chcd2-Dzr_cl_chcd2 * clzr-Dzz_cl_chcd2 * clzz+clz * v_cl_chcd2-R_cl_chcd2)
res_sc_cl_chcd2	Shock capturing residual for cl	mol/(m^2*s)	r * (clr * u_cl_chcd2+clz * v_cl_chcd2-R_cl_chcd2)
da_cl_chcd2	Total time scale	m	r * Dts_cl_chcd2

	factor, cl		

9 Appendix 3: Mini-Absorber, Lumped Parameter Model for Absorption/Reaction

COMSOL Model Report



1. Table of Contents

2. Model Properties

Property	Value
Model name	
Author	
Company	
Department	
Reference	
URL	
Saved date	Apr 16, 2009 9:51:35 PM
Creation date	Jun 11, 2008 1:16:28 PM
COMSOL version	COMSOL 3.5.0.603

File name: R:\Absorption\absorber-mini-rxn.mph

Application modes and modules used in this model:

- Geom1 (Axial symmetry (2D))

- Convection and Diffusion (Chemical Engineering Module)
- Convection and Diffusion (Chemical Engineering Module)
- Convection and Diffusion (Chemical Engineering Module)

3. Constants

Name	Expression	Value	Description
W	.01		
A	1.5		air rate in (L/min)
yin	.178		mole fraction CO2 in
Kh	614.26*W+212.25		mass trans coeff (mol/m3h)
H	1420		Henrys constant (atm)
Ka	Kh/3600		mass trans coeff (mol/m3s)
vl	-(W*1000/100^3/60/4.56e-3)		liquid velocity (m/s)
vgo	A*1000/100^3/60/4.56e-3		air velocity in (m/s)
cl0	0		liquid CO2 conc. in (mol/m3)
cg0	yin*101325/8.314/273		gas CO2 conc. in (mol/m3)
Dg	1.6e-5		diff. coeff. gas (m2/s)
Dl	1.8e-9		diff. coeff. liquid (m2./s)
cna0	1000		
coh0	1000		
cco30	0		
Temp	295		
K	6.7772*W^0.86		

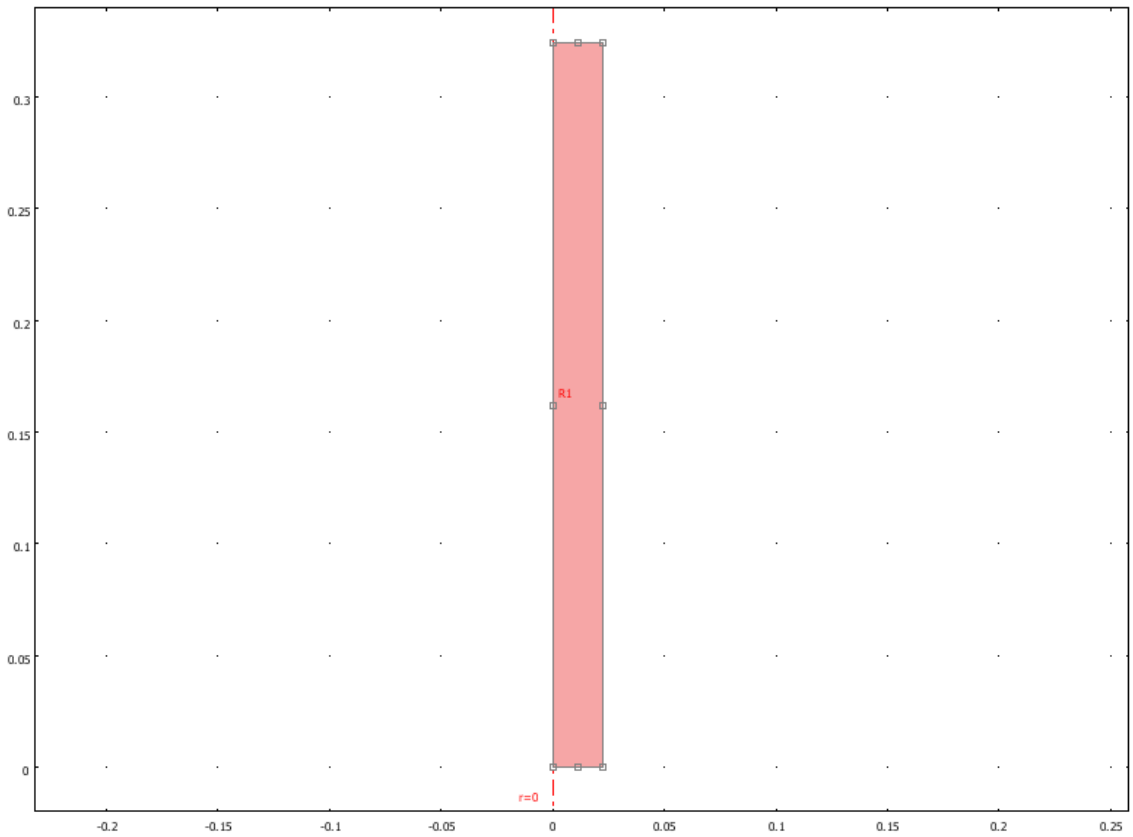
4. Global Expressions

Name	Expression	Unit	Description
y	cg*8.314*273/101325	mol/m^3	
x	cl*1000/55.55/100^3	mol/m^3	
ye	H*x	mol/m^3	
vg	vgo/(1-y)	m^3/mol	
I	1/2*(cna+coh+cco3*4)[m^3/mol]	1	
logk	11.895-2382/Temp+0.221*I/1000-0.016*(I/1000)^2	1	
kb	exp(logk)[m^3/mol/s]/1000	m^3/(s*mol)	

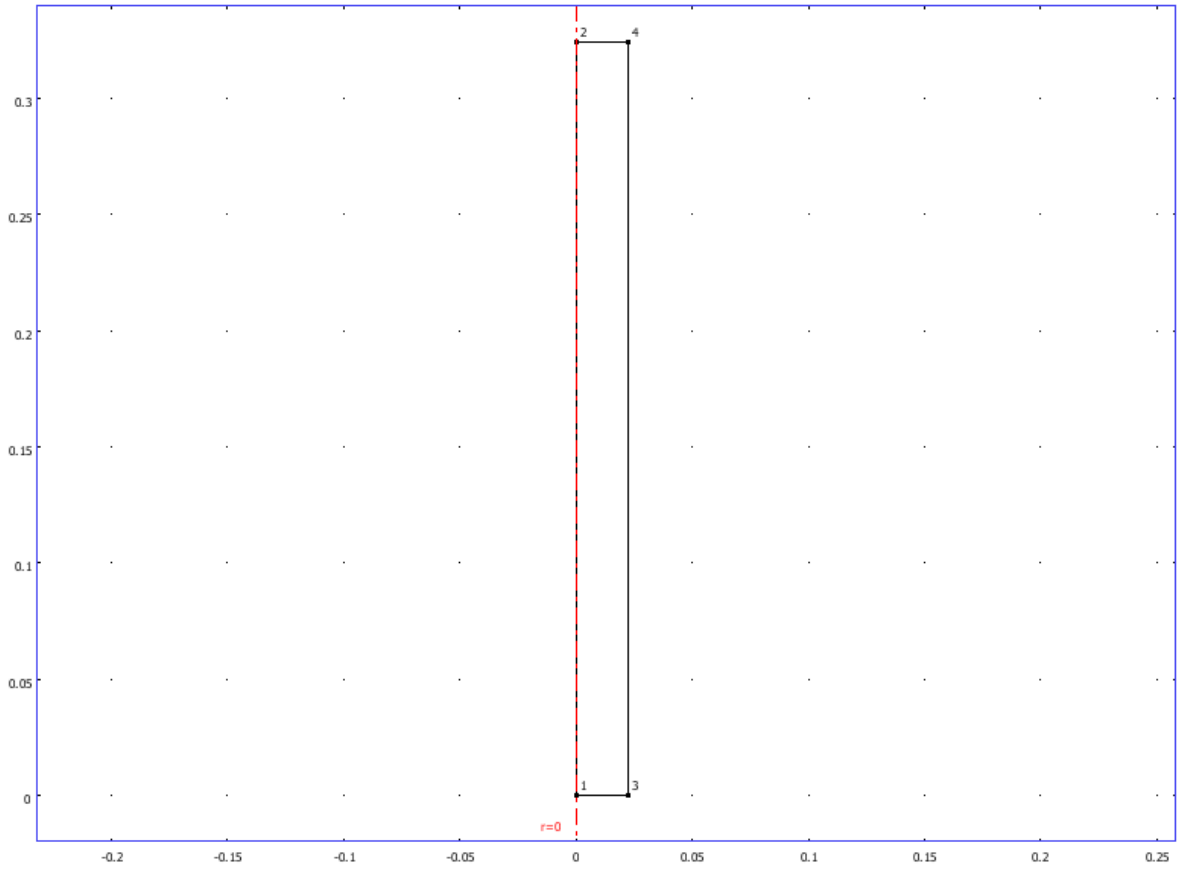
5. Geometry

Number of geometries: 1

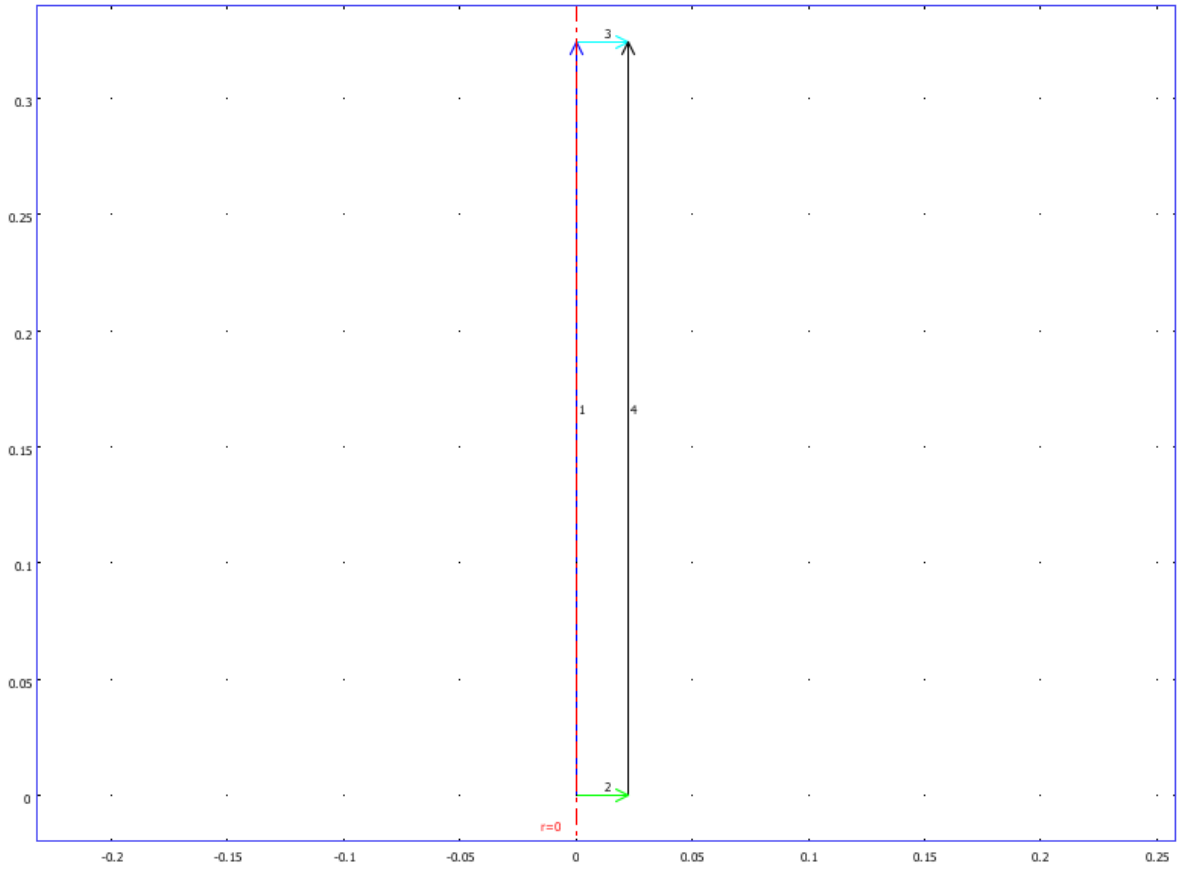
5.1. Geom1



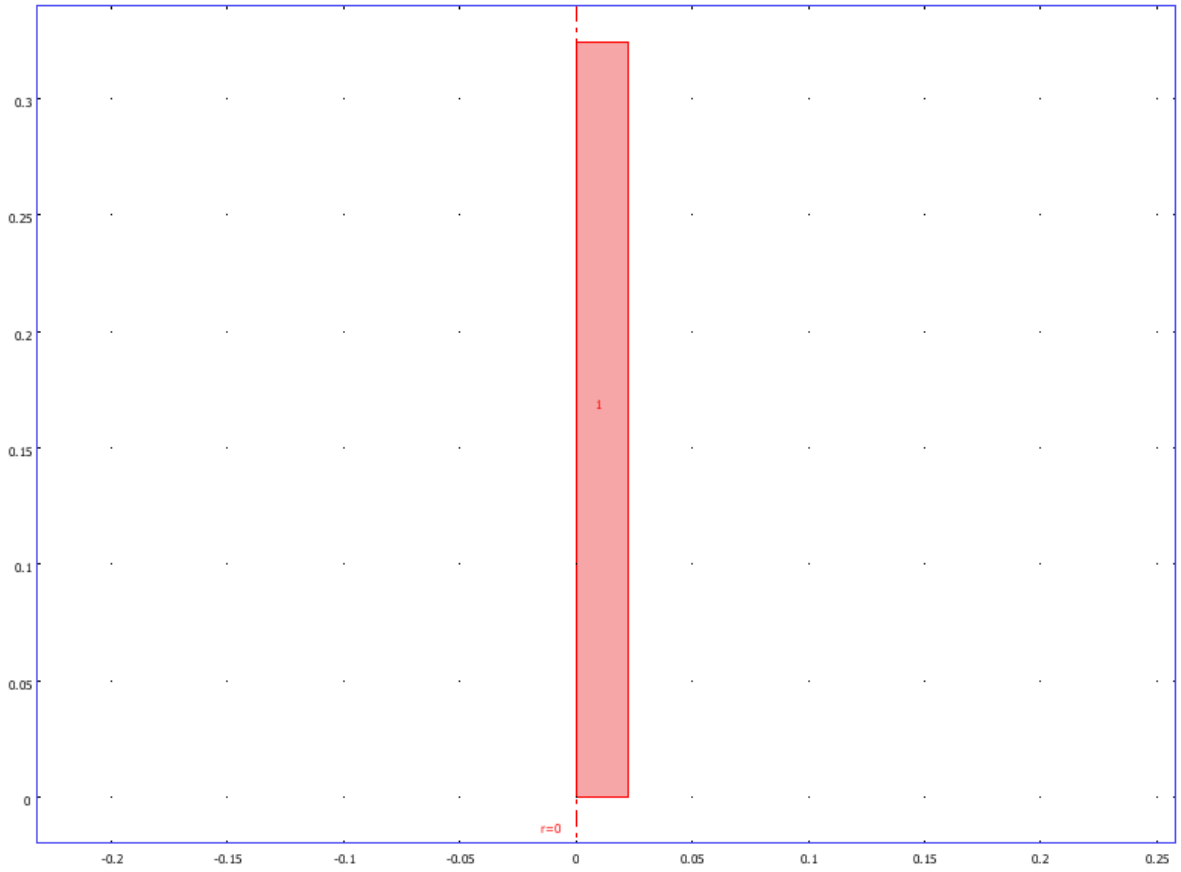
5.1.1. Point mode



5.1.2. Boundary mode



5.1.3. Subdomain mode



6. Geom1

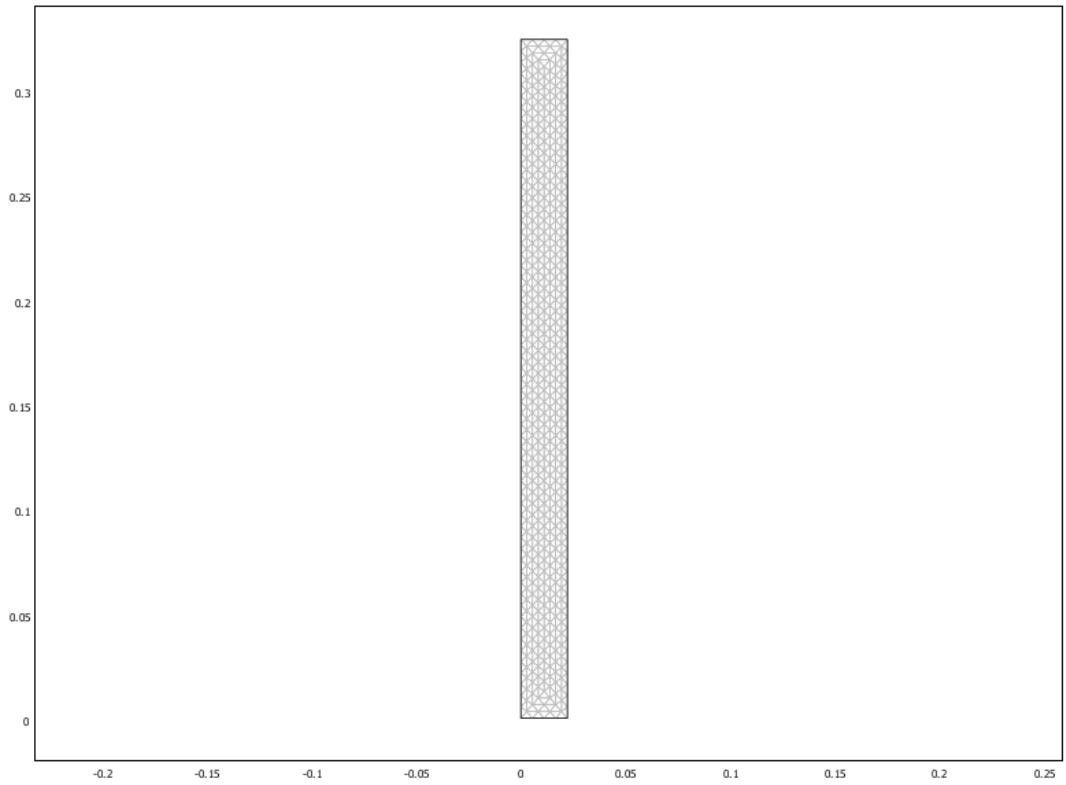
Space dimensions: Axial symmetry (2D)

Independent variables: r, phi, z

6.1. Mesh

6.1.1. Mesh Statistics

Number of degrees of freedom	10245
Number of mesh points	545
Number of elements	960
Triangular	960
Quadrilateral	0
Number of boundary elements	128
Number of vertex elements	4
Minimum element quality	0.87
Element area ratio	0.75



6.2. Application Mode: Convection and Diffusion (chcd)

Application mode type: Convection and Diffusion (Chemical Engineering Module)

Application mode name: chcd

6.2.1. Application Mode Properties

Property	**Value**
Default element type	Lagrange - Quadratic
Analysis type	Stationary
Equation form	Non-conservative
Equilibrium assumption	Off
Frame	Frame (ref)
Weak constraints	Off
Constraint type	Ideal

6.2.2. Variables

Dependent variables: cg

Shape functions: shlag(2,'cg')

Interior boundaries not active

6.2.3. Boundary Settings

Boundary		1	2	3
Type		Axial symmetry	Concentration	Convective flux
Concentration (c0)	mol/m^3	0	**cg0**	0

Boundary		4
Type		Insulation/Symmetry
Concentration (c0)	mol/m^3	0

6.2.4. Subdomain Settings

Subdomain		1
Diffusion coefficient (D)	m^2/s	**Dg**
Reaction rate (R)	$mol/(m^3 \cdot s)$	**-K*(y-ye)**
z-velocity (v)	m/s	**vg**

6.3. Application Mode: Convection and Diffusion (chcd2)

Application mode type: Convection and Diffusion (Chemical Engineering Module)

Application mode name: chcd2

6.3.1. Application Mode Properties

Property	**Value**
Default element type	Lagrange - Quadratic
Analysis type	Stationary
Equation form	Non-conservative
Equilibrium assumption	Off
Frame	Frame (ref)
Weak constraints	Off
Constraint type	Ideal

6.3.2. Variables

Dependent variables: cl

Shape functions: shlag(2,'cl')

Interior boundaries not active

6.3.3. Boundary Settings

Boundary		1	2	3

Type		Axial symmetry	Convective flux	Concentration
Concentration (c0)	mol/m^3	0	0	**cl0**

Boundary		4
Type		Insulation/Symmetry
Concentration (c0)	mol/m^3	0

6.3.4. Subdomain Settings

Subdomain		1
Diffusion coefficient (D)	m^2/s	**Dl**
Reaction rate (R)	$mol/(m^3 \cdot s)$	**K*(y-ye)-kb*cl**
z-velocity (v)	m/s	**vl**

6.4. Application Mode: Convection and Diffusion (chcd3)

Application mode type: Convection and Diffusion (Chemical Engineering Module)

Application mode name: chcd3

6.4.1. Application Mode Properties

Property	**Value**
Default element type	Lagrange - Quadratic
Analysis type	Stationary
Equation form	Non-conservative
Equilibrium assumption	Off
Frame	Frame (ref)
Weak constraints	Off
Constraint type	Ideal

6.4.2. Variables

Dependent variables: cna, coh, cco3

Shape functions: shlag(2,'cna'), shlag(2,'coh'), shlag(2,'cco3')

Interior boundaries not active

6.4.3. Boundary Settings

Boundary		1, 4	2	3
Type		Insulation/Symmetry	Convective flux	Concentration
Concentration (c0)	mol/m^3	{0;0;0}	{0;0;0}	**{cna0;coh0;cco30}**

6.4.4. Subdomain Settings

Subdomain		1
Diffusion coefficient (D)	m^2/s	**{Dl*1.7;Dl*1.7;Dl*1.7}**
Reaction rate (R)	$mol/(m^3 \cdot s)$	**{0;-kb*cl*coh;kb*cl*coh}**
z-velocity (v)	m/s	**{vl;vl;vl}**

7. Solver Settings

Solve using a script: off

Analysis type	Stationary
Auto select solver	On
Solver	Parametric
Solution form	Automatic
Symmetric	auto
Adaptive mesh refinement	Off
Optimization/Sensitivity	Off
Plot while solving	Off

7.1. Direct (UMFPACK)

Solver type: Linear system solver

Parameter	**Value**
Pivot threshold	0.1
Memory allocation factor	0.7

7.2. Stationary

Parameter	**Value**
Linearity	Automatic
Relative tolerance	1.0E-6
Maximum number of iterations	25
Manual tuning of damping parameters	Off
Highly nonlinear problem	Off
Initial damping factor	1.0
Minimum damping factor	1.0E-4
Restriction for step size update	10.0

7.3. Parametric

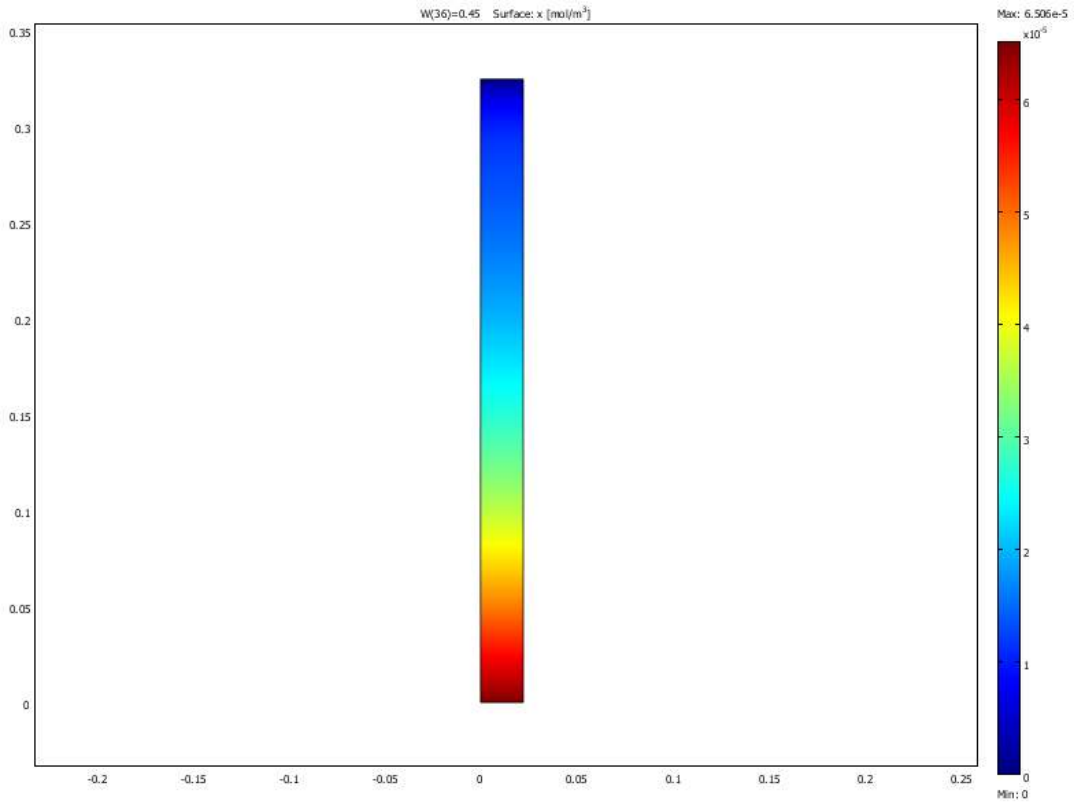
Parameter	**Value**
Parameter name	W

Parameter values	range(0.1,0.01,0.45)
Predictor	Linear
Manual tuning of parameter step size	Off
Initial step size	0.0
Minimum step size	0.0
Maximum step size	0.0

7.4. Advanced

Parameter	**Value**
Constraint handling method	Elimination
Null-space function	Automatic
Automatic assembly block size	On
Assembly block size	5000
Use Hermitian transpose of constraint matrix and in symmetry detection	Off
Use complex functions with real input	Off
Stop if error due to undefined operation	On
Store solution on file	Off
Type of scaling	Automatic
Manual scaling	
Row equilibration	On
Manual control of reassembly	Off
Load constant	On
Constraint constant	On
Mass constant	On
Damping (mass) constant	On
Jacobian constant	On
Constraint Jacobian constant	On

8. Postprocessing



9. Variables

9.1. Boundary

Name	Description	Unit	Expression
ndflux_cg_chcd	Normal diffusive flux, cg	mol/(m^2*s)	nr_chcd * dflux_cg_r_chcd+nz_chcd * dflux_cg_z_chcd
ncflux_cg_chcd	Normal convective flux, cg	mol/(m^2*s)	nr_chcd * cflux_cg_r_chcd+nz_chcd * cflux_cg_z_chcd
ntflux_cg_chcd	Normal total flux, cg	mol/(m^2*s)	nr_chcd * tflux_cg_r_chcd+nz_chcd * tflux_cg_z_chcd
ndflux_cl_chcd2	Normal diffusive flux, cl	mol/(m^2*s)	nr_chcd2 * dflux_cl_r_chcd2+nz_chcd2 * dflux_cl_z_chcd2
ncflux_cl_chcd2	Normal convective flux, cl	mol/(m^2*s)	nr_chcd2 * cflux_cl_r_chcd2+nz_chcd2 * cflux_cl_z_chcd2
ntflux_cl_chcd2	Normal total flux, cl	mol/(m^2*s)	nr_chcd2 * tflux_cl_r_chcd2+nz_chcd2 * tflux_cl_z_chcd2
ndflux_cna_chcd3	Normal	mol/(m^2*s)	nr_chcd3 *

	diffusive flux, cna		dflux_cna_r_chcd3+nz_chcd3 * dflux_cna_z_chcd3
ncflux_cna_chcd3	Normal convective flux, cna	mol/(m^2*s)	nr_chcd3 * cflux_cna_r_chcd3+nz_chcd3 * cflux_cna_z_chcd3
ntflux_cna_chcd3	Normal total flux, cna	mol/(m^2*s)	nr_chcd3 * tflux_cna_r_chcd3+nz_chcd3 * tflux_cna_z_chcd3
ndflux_coh_chcd3	Normal diffusive flux, coh	mol/(m^2*s)	nr_chcd3 * dflux_coh_r_chcd3+nz_chcd3 * dflux_coh_z_chcd3
ncflux_coh_chcd3	Normal convective flux, coh	mol/(m^2*s)	nr_chcd3 * cflux_coh_r_chcd3+nz_chcd3 * cflux_coh_z_chcd3
ntflux_coh_chcd3	Normal total flux, coh	mol/(m^2*s)	nr_chcd3 * tflux_coh_r_chcd3+nz_chcd3 * tflux_coh_z_chcd3
ndflux_cco3_chcd3	Normal diffusive flux, cco3	mol/(m^2*s)	nr_chcd3 * dflux_cco3_r_chcd3+nz_chcd3 * dflux_cco3_z_chcd3
ncflux_cco3_chcd3	Normal convective flux, cco3	mol/(m^2*s)	nr_chcd3 * cflux_cco3_r_chcd3+nz_chcd3 * cflux_cco3_z_chcd3
ntflux_cco3_chcd3	Normal total flux, cco3	mol/(m^2*s)	nr_chcd3 * tflux_cco3_r_chcd3+nz_chcd3 * tflux_cco3_z_chcd3

9.2. Subdomain

Name	**Description**	**Unit**	**Expression**
grad_cg_r_chcd	Concentration gradient, cg, r component	mol/m^4	cgr
dflux_cg_r_chcd	Diffusive flux, cg, r component	mol/(m^2*s)	-Drr_cg_chcd * cgr-Drz_cg_chcd * cgz
cflux_cg_r_chcd	Convective flux, cg, r	mol/(m^2*s)	cg * u_cg_chcd

	component		
tflux_cg_r_chcd	Total flux, cg, r component	mol/(m^2*s)	dflux_cg_r_chcd+cflux_cg_r_chcd
grad_cg_z_chcd	Concentration gradient, cg, z component	mol/m^4	cgz
dflux_cg_z_chcd	Diffusive flux, cg, z component	mol/(m^2*s)	-Dzr_cg_chcd * cgr-Dzz_cg_chcd * cgz
cflux_cg_z_chcd	Convective flux, cg, z component	mol/(m^2*s)	cg * v_cg_chcd
tflux_cg_z_chcd	Total flux, cg, z component	mol/(m^2*s)	dflux_cg_z_chcd+cflux_cg_z_chcd
beta_cg_r_chcd	Convective field, cg, r component	m^2/s	r * u_cg_chcd
beta_cg_z_chcd	Convective field, cg, z component	m^2/s	r * v_cg_chcd
grad_cg_chcd	Concentration gradient, cg	mol/m^4	sqrt(grad_cg_r_chcd^2+grad_cg_z_chcd^2)
dflux_cg_chcd	Diffusive flux, cg	mol/(m^2*s)	sqrt(dflux_cg_r_chcd^2+dflux_cg_z_chcd^2)
cflux_cg_chcd	Convective flux, cg	mol/(m^2*s)	sqrt(cflux_cg_r_chcd^2+cflux_cg_z_chcd^2)

tflux_cg_chcd	Total flux, cg	mol/(m^2*s)	sqrt(tflux_cg_r_chcd^2+tflux_cg_z_chcd^2)
cellPe_cg_chcd	Cell Peclet number, cg	1	h * sqrt(beta_cg_r_chcd^2+beta_cg_z_chcd^2)/Dm_cg_chcd
Dm_cg_chcd	Mean diffusion coefficient, cg	m^3/s	r * (Drr_cg_chcd * u_cg_chcd^2+Drz_cg_chcd * u_cg_chcd * v_cg_chcd+Dzr_cg_chcd * v_cg_chcd * u_cg_chcd+Dzz_cg_chcd * v_cg_chcd^2)/(u_cg_chcd^2+v_cg_chcd^2+eps)
res_cg_chcd	Equation residual for cg	mol/(m^2*s)	r * (-Drr_cg_chcd * cgrr-Drz_cg_chcd * cgrz+cgr * u_cg_chcd-Dzr_cg_chcd * cgzr-Dzz_cg_chcd * cgzz+cgz * v_cg_chcd-R_cg_chcd)
res_sc_cg_chcd	Shock capturing residual for cg	mol/(m^2*s)	r * (cgr * u_cg_chcd+cgz * v_cg_chcd-R_cg_chcd)
da_cg_chcd	Total time scale factor, cg	m	r * Dts_cg_chcd
grad_cl_r_chcd2	Concentration gradient, cl, r component	mol/m^4	clr
dflux_cl_r_chcd2	Diffusive flux, cl, r component	mol/(m^2*s)	-Drr_cl_chcd2 * clr-Drz_cl_chcd2 * clz
cflux_cl_r_chcd2	Convective flux, cl, r component	mol/(m^2*s)	cl * u_cl_chcd2
tflux_cl_r_chcd2	Total flux, cl, r component	mol/(m^2*s)	dflux_cl_r_chcd2+cflux_cl_r_chcd2
grad_cl_z_chcd2	Concentration gradient, cl, z	mol/m^4	clz

	component		
dflux_cl_z_chcd2	Diffusive flux, cl, z component	mol/(m^2*s)	-Dzr_cl_chcd2 * clr-Dzz_cl_chcd2 * clz
cflux_cl_z_chcd2	Convective flux, cl, z component	mol/(m^2*s)	cl * v_cl_chcd2
tflux_cl_z_chcd2	Total flux, cl, z component	mol/(m^2*s)	dflux_cl_z_chcd2+cflux_cl_z_chcd2
beta_cl_r_chcd2	Convective field, cl, r component	m^2/s	r * u_cl_chcd2
beta_cl_z_chcd2	Convective field, cl, z component	m^2/s	r * v_cl_chcd2
grad_cl_chcd2	Concentration gradient, cl	mol/m^4	sqrt(grad_cl_r_chcd2^2+grad_cl_z_chcd2^2)
dflux_cl_chcd2	Diffusive flux, cl	mol/(m^2*s)	sqrt(dflux_cl_r_chcd2^2+dflux_cl_z_chcd2^2)
cflux_cl_chcd2	Convective flux, cl	mol/(m^2*s)	sqrt(cflux_cl_r_chcd2^2+cflux_cl_z_chcd2^2)
tflux_cl_chcd2	Total flux, cl	mol/(m^2*s)	sqrt(tflux_cl_r_chcd2^2+tflux_cl_z_chcd2^2)
cellPe_cl_chcd2	Cell Peclet number, cl	1	h * sqrt(beta_cl_r_chcd2^2+beta_cl_z_chcd2^2)/Dm_cl_chcd2
Dm_cl_chcd2	Mean diffusion coefficien	m^3/s	r * (Drr_cl_chcd2 * u_cl_chcd2^2+Drz_cl_chcd2 * u_cl_chcd2 * v_cl_chcd2+Dzr_cl_chcd2 * v_cl_chcd2 * u_cl_chcd2+Dzz_cl_chcd2 *

	t, cl		v_cl_chcd2^2)/(u_cl_chcd2^2+v_cl_chcd2^2+eps)
res_cl_chcd2	Equation residual for cl	mol/(m^2*s)	r * (-Drr_cl_chcd2 * clrr-Drz_cl_chcd2 * clrz+clr * u_cl_chcd2-Dzr_cl_chcd2 * clzr-Dzz_cl_chcd2 * clzz+clz * v_cl_chcd2-R_cl_chcd2)
res_sc_cl_chcd2	Shock capturing residual for cl	mol/(m^2*s)	r * (clr * u_cl_chcd2+clz * v_cl_chcd2-R_cl_chcd2)
da_cl_chcd2	Total time scale factor, cl	m	r * Dts_cl_chcd2
grad_cna_r_chcd3	Concentration gradient, cna, r component	mol/m^4	cnar
dflux_cna_r_chcd3	Diffusive flux, cna, r component	mol/(m^2*s)	-Drr_cna_chcd3 * cnar-Drz_cna_chcd3 * cnaz
cflux_cna_r_chcd3	Convective flux, cna, r component	mol/(m^2*s)	cna * u_cna_chcd3
tflux_cna_r_chcd3	Total flux, cna, r component	mol/(m^2*s)	dflux_cna_r_chcd3+cflux_cna_r_chcd3
grad_cna_z_chcd3	Concentration gradient, cna, z component	mol/m^4	cnaz
dflux_cna_z_chcd3	Diffusive flux, cna, z component	mol/(m^2*s)	-Dzr_cna_chcd3 * cnar-Dzz_cna_chcd3 * cnaz
cflux_cna_z_c	Convectiv	mol/(m^	cna * v_cna_chcd3

hcd3	e flux, cna, z componen t	2*s)	
tflux_cna_z_ch cd3	Total flux, cna, z componen t	mol/(m^ 2*s)	dflux_cna_z_chcd3+cflux_cna_z_chcd3
beta_cna_r_ch cd3	Convectiv e field, cna, r componen t	m^2/s	r * u_cna_chcd3
beta_cna_z_ch cd3	Convectiv e field, cna, z componen t	m^2/s	r * v_cna_chcd3
grad_cna_chcd 3	Concentra tion gradient, cna	mol/m^4	sqrt(grad_cna_r_chcd3^2+grad_cna_z_chcd3^2)
dflux_cna_chc d3	Diffusive flux, cna	mol/(m^ 2*s)	sqrt(dflux_cna_r_chcd3^2+dflux_cna_z_chcd3^2)
cflux_cna_chc d3	Convectiv e flux, cna	mol/(m^ 2*s)	sqrt(cflux_cna_r_chcd3^2+cflux_cna_z_chcd3^2)
tflux_cna_chcd 3	Total flux, cna	mol/(m^ 2*s)	sqrt(tflux_cna_r_chcd3^2+tflux_cna_z_chcd3^2)
cellPe_cna_chc d3	Cell Peclet number, cna	1	h * sqrt(beta_cna_r_chcd3^2+beta_cna_z_chcd3^2)/D m_cna_chcd3
Dm_cna_chcd 3	Mean diffusion coefficien t, cna	m^3/s	r * (Drr_cna_chcd3 * u_cna_chcd3^2+Drz_cna_chcd3 * u_cna_chcd3 * v_cna_chcd3+Dzr_cna_chcd3 * v_cna_chcd3 * u_cna_chcd3+Dzz_cna_chcd3 * v_cna_chcd3^2)/(u_cna_chcd3^2+v_cna_chcd3^2 +eps)
res_cna_chcd3	Equation residual for cna	mol/(m^ 2*s)	r * (-Drr_cna_chcd3 * cnarr-Drz_cna_chcd3 * cnarz+cnar * u_cna_chcd3-Dzr_cna_chcd3 * cnazr-Dzz_cna_chcd3 * cnazz+cnaz * v_cna_chcd3-R_cna_chcd3)

res_sc_cna_chcd3	Shock capturing residual for cna	mol/(m^2*s)	r * (cnar * u_cna_chcd3+cnaz * v_cna_chcd3-R_cna_chcd3)
da_cna_chcd3	Total time scale factor, cna	m	r * Dts_cna_chcd3
grad_coh_r_chcd3	Concentration gradient, coh, r component	mol/m^4	cohr
dflux_coh_r_chcd3	Diffusive flux, coh, r component	mol/(m^2*s)	-Drr_coh_chcd3 * cohr-Drz_coh_chcd3 * cohz
cflux_coh_r_chcd3	Convective flux, coh, r component	mol/(m^2*s)	coh * u_coh_chcd3
tflux_coh_r_chcd3	Total flux, coh, r component	mol/(m^2*s)	dflux_coh_r_chcd3+cflux_coh_r_chcd3
grad_coh_z_chcd3	Concentration gradient, coh, z component	mol/m^4	cohz
dflux_coh_z_chcd3	Diffusive flux, coh, z component	mol/(m^2*s)	-Dzr_coh_chcd3 * cohr-Dzz_coh_chcd3 * cohz
cflux_coh_z_chcd3	Convective flux, coh, z component	mol/(m^2*s)	coh * v_coh_chcd3

tflux_coh_z_chcd3	Total flux, coh, z component	mol/(m^2*s)	dflux_coh_z_chcd3+cflux_coh_z_chcd3
beta_coh_r_chcd3	Convective field, coh, r component	m^2/s	r * u_coh_chcd3
beta_coh_z_chcd3	Convective field, coh, z component	m^2/s	r * v_coh_chcd3
grad_coh_chcd3	Concentration gradient, coh	mol/m^4	sqrt(grad_coh_r_chcd3^2+grad_coh_z_chcd3^2)
dflux_coh_chcd3	Diffusive flux, coh	mol/(m^2*s)	sqrt(dflux_coh_r_chcd3^2+dflux_coh_z_chcd3^2)
cflux_coh_chcd3	Convective flux, coh	mol/(m^2*s)	sqrt(cflux_coh_r_chcd3^2+cflux_coh_z_chcd3^2)
tflux_coh_chcd3	Total flux, coh	mol/(m^2*s)	sqrt(tflux_coh_r_chcd3^2+tflux_coh_z_chcd3^2)
cellPe_coh_chcd3	Cell Peclet number, coh	1	h * sqrt(beta_coh_r_chcd3^2+beta_coh_z_chcd3^2)/Dm_coh_chcd3
Dm_coh_chcd3	Mean diffusion coefficient, coh	m^3/s	r * (Drr_coh_chcd3 * u_coh_chcd3^2+Drz_coh_chcd3 * u_coh_chcd3 * v_coh_chcd3+Dzr_coh_chcd3 * v_coh_chcd3 * u_coh_chcd3+Dzz_coh_chcd3 * v_coh_chcd3^2)/(u_coh_chcd3^2+v_coh_chcd3^2+eps)
res_coh_chcd3	Equation residual for coh	mol/(m^2*s)	r * (-Drr_coh_chcd3 * cohrr-Drz_coh_chcd3 * cohrz+cohr * u_coh_chcd3-Dzr_coh_chcd3 * cohzr-Dzz_coh_chcd3 * cohzz+cohz * v_coh_chcd3-R_coh_chcd3)
res_sc_coh_chcd3	Shock capturing residual for coh	mol/(m^2*s)	r * (cohr * u_coh_chcd3+cohz * v_coh_chcd3-R_coh_chcd3)

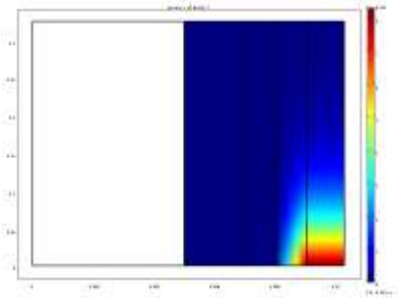
da_coh_chcd3	Total time scale factor, coh	m	r * Dts_coh_chcd3
grad_cco3_r_chcd3	Concentration gradient, cco3, r component	mol/m^4	cco3r
dflux_cco3_r_chcd3	Diffusive flux, cco3, r component	mol/(m^2*s)	-Drr_cco3_chcd3 * cco3r-Drz_cco3_chcd3 * cco3z
cflux_cco3_r_chcd3	Convective flux, cco3, r component	mol/(m^2*s)	cco3 * u_cco3_chcd3
tflux_cco3_r_chcd3	Total flux, cco3, r component	mol/(m^2*s)	dflux_cco3_r_chcd3+cflux_cco3_r_chcd3
grad_cco3_z_chcd3	Concentration gradient, cco3, z component	mol/m^4	cco3z
dflux_cco3_z_chcd3	Diffusive flux, cco3, z component	mol/(m^2*s)	-Dzr_cco3_chcd3 * cco3r-Dzz_cco3_chcd3 * cco3z
cflux_cco3_z_chcd3	Convective flux, cco3, z component	mol/(m^2*s)	cco3 * v_cco3_chcd3
tflux_cco3_z_chcd3	Total flux, cco3, z componen	mol/(m^2*s)	dflux_cco3_z_chcd3+cflux_cco3_z_chcd3

	t		
beta_cco3_r_chcd3	Convective field, cco3, r component	m^2/s	r * u_cco3_chcd3
beta_cco3_z_chcd3	Convective field, cco3, z component	m^2/s	r * v_cco3_chcd3
grad_cco3_chcd3	Concentration gradient, cco3	mol/m^4	sqrt(grad_cco3_r_chcd3^2+grad_cco3_z_chcd3^2)
dflux_cco3_chcd3	Diffusive flux, cco3	mol/(m^2*s)	sqrt(dflux_cco3_r_chcd3^2+dflux_cco3_z_chcd3^2)
cflux_cco3_chcd3	Convective flux, cco3	mol/(m^2*s)	sqrt(cflux_cco3_r_chcd3^2+cflux_cco3_z_chcd3^2)
tflux_cco3_chcd3	Total flux, cco3	mol/(m^2*s)	sqrt(tflux_cco3_r_chcd3^2+tflux_cco3_z_chcd3^2)
cellPe_cco3_chcd3	Cell Peclet number, cco3	1	h * sqrt(beta_cco3_r_chcd3^2+beta_cco3_z_chcd3^2) /Dm_cco3_chcd3
Dm_cco3_chcd3	Mean diffusion coefficient, cco3	m^3/s	r * (Drr_cco3_chcd3 * u_cco3_chcd3^2+Drz_cco3_chcd3 * u_cco3_chcd3 * v_cco3_chcd3+Dzr_cco3_chcd3 * v_cco3_chcd3 * u_cco3_chcd3+Dzz_cco3_chcd3 * v_cco3_chcd3^2)/(u_cco3_chcd3^2+v_cco3_chcd3^2+eps)
res_cco3_chcd3	Equation residual for cco3	mol/(m^2*s)	r * (-Drr_cco3_chcd3 * cco3rr-Drz_cco3_chcd3 * cco3rz+cco3r * u_cco3_chcd3-Dzr_cco3_chcd3 * cco3zr-Dzz_cco3_chcd3 * cco3zz+cco3z * v_cco3_chcd3-R_cco3_chcd3)
res_sc_cco3_chcd3	Shock capturing residual for cco3	mol/(m^2*s)	r * (cco3r * u_cco3_chcd3+cco3z * v_cco3_chcd3-R_cco3_chcd3)
da_cco3_chcd3	Total time	m	r * Dts_cco3_chcd3

	scale factor, cco3		

10 Appendix 4: Mini-Absorber, Two-Film Model for Absorption with Reaction

COMSOL Model Report



1. Table of Contents

2. Model Properties

Property	Value
Model name	
Author	
Company	
Department	
Reference	
URL	
Saved date	Apr 23, 2009 2:32:58 PM
Creation date	Apr 18, 2008 1:31:23 PM
COMSOL version	COMSOL 3.5.0.603

File name: R:\Absorption\absorber-micro-mini-rxn.mph

Application modes and modules used in this model:

- Geom1 (Axial symmetry (2D))

- Convection and Diffusion (Chemical Engineering Module)
- Convection and Diffusion (Chemical Engineering Module)
- Convection and Diffusion (Chemical Engineering Module)

3. Constants

Name	Expression	Value	Description
W	.3	0.3	water rate in (L/min)
A	1.42	1.42	air rate in (L/min)
yin	0.185	0.185	mole fraction CO2 in
Kh	0.1706*W+0.059	0.11018	overall mass transfer coefficient (mol/m3h)
H	1420	1420	Henrys constant (atm)
Z	1.372	1.372	packing height (m)
S	0.00456	0.00456	column cross sectional area (m2)
vl	-(W*1000/100^3/60/S)	-0.001096	liquid velocity (m/s)
r1	0.005	0.005	radius of glass rod (m)
tfl	0.002	0.002	thicknes of flowing liquid layer (m)
tfilm	0.001	0.001	model stagnant film thickness (m)
Alfilm	pi*((r1+tfl)^2-r1^2)	7.539822e-5	area of liquid film (m2)
NR	S/Alfilm	60.478878	number of glass rods
vgo	A*1000/100^3/60/S	0.00519	air velocity (m/s)
vgin	vgo/(1-yin)	0.006368	gas velocity in (m/s)
Agfilm	S/NR	7.539822e-5	area of gas film (m2)
tfg	(Agfilm/pi+(r1+tfl+2*tfilm)^2)^0.5-(r1+tfl+2*tfilm)	0.001247	thickness of flowing gas layer (m)
cl0	0	0	liquid CO2 conc. in (mol/m3)
cg0	yin*101325/8.314/273	8.258776	gas CO2 conc. in (mol/m3)
Dg	1.6e-5	1.6e-5	diff. coeff. gas (m2/s)
Dl	1.8e-9	1.8e-9	diff. coeff. liquid (m2/s)
V	S*Z	0.006256	column volume (m3)
kya	1/(0.2812*W^-0.5-0.2706)	4.11864	gas side mass trans

			coeff (mol/m3s)
Kya	Kh/3600	3.060556e-5	overall mass trans coeff (mol/m3s)
kxa	1000000	10e5	liquid side mass trans coeff (mol/m3s)
ia	Z*2*pi*(r1+tfl+tfilm)*NR	4.17088	total interfacial area (m2)
a	ia/V	666.666667	interfacial area per volume (m2/m3)
Deffg	kya/a*tfilm/(101325/(8.314*273))	1.383889e-7	Effective diffusivity in gas film (m2/s)
Deffl	kxa/a*tfilm/(55.556*100^3/1000)	2.699978e-5	Effective diffusivity in liquid film (m2/s)
yout	0.099	0.099	mole fraction CO2 out
vgout	vgo/(1-yout)	0.00576	gas velocity out (m/s)
vgave	(vgin+vgout)/2	0.006064	average gas velocity (m/s)
M	10000	10000	Stiff spring constant
tl	Dl*tfilm/Deffl	6.66672e-8	predicted stagnant liquid film thickness (m)
Cna0	1000	1000	liquid Na+ conc. in (mol/m3)
Cco30	0	0	liquid CO3-2 conc in. (mol/m3)
Coh0	2*Cna0	2000	liquid OH- conc. in (mol/m3)
Temp	298	298	

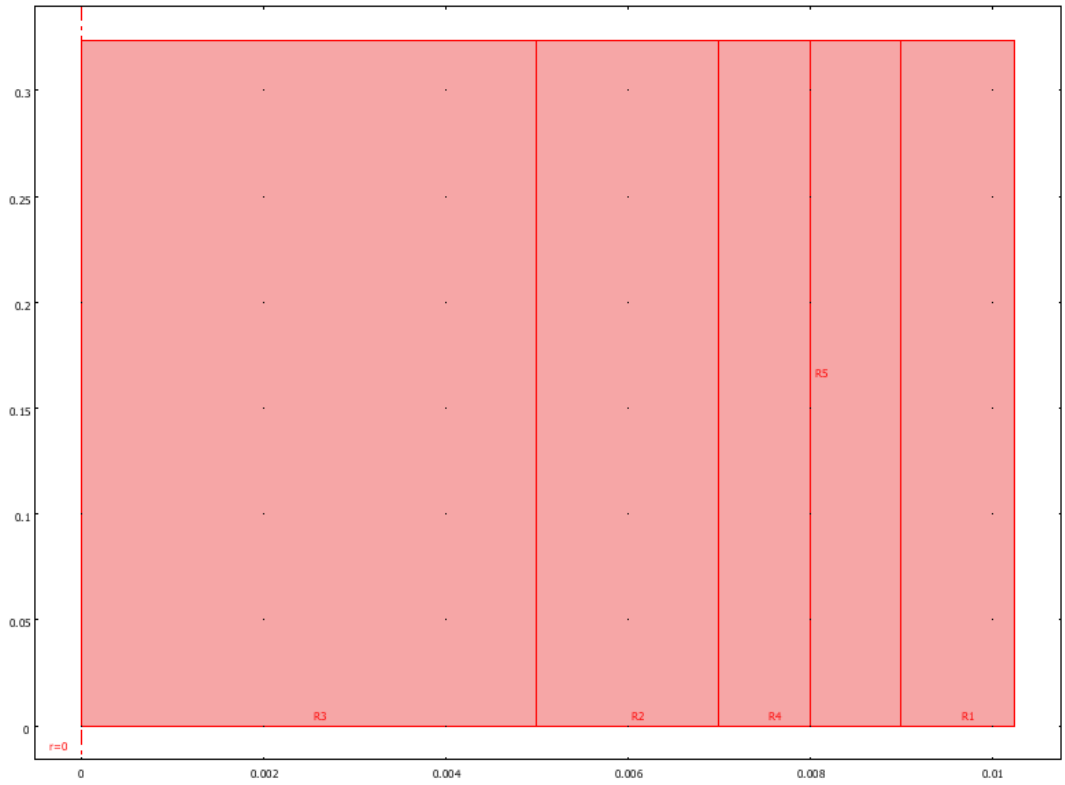
4. Global Expressions

Name	Expression	Unit	Description
y	cg*8.314*273/101325	mol/m^3	
x	cl*1000/55.55/100^3	mol/m^3	
vg	vgo/(1-y)	m^3/mol	
ye	H*x	mol/m^3	

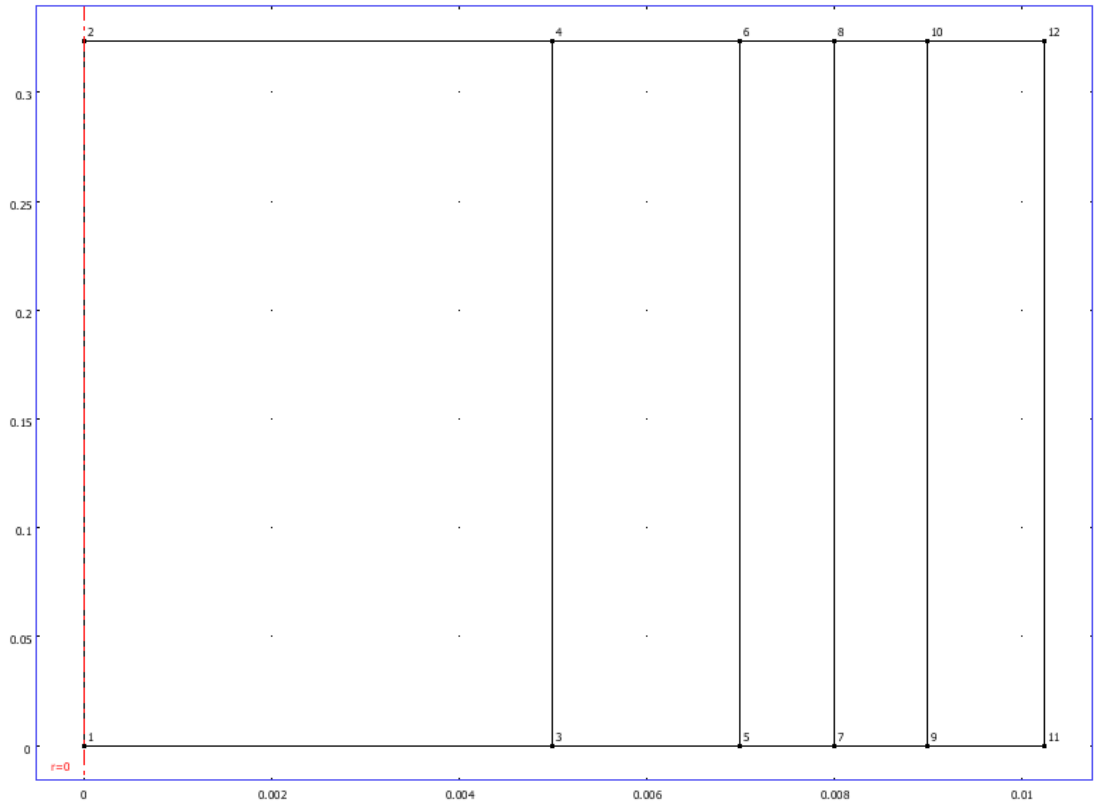
5. Geometry

Number of geometries: 1

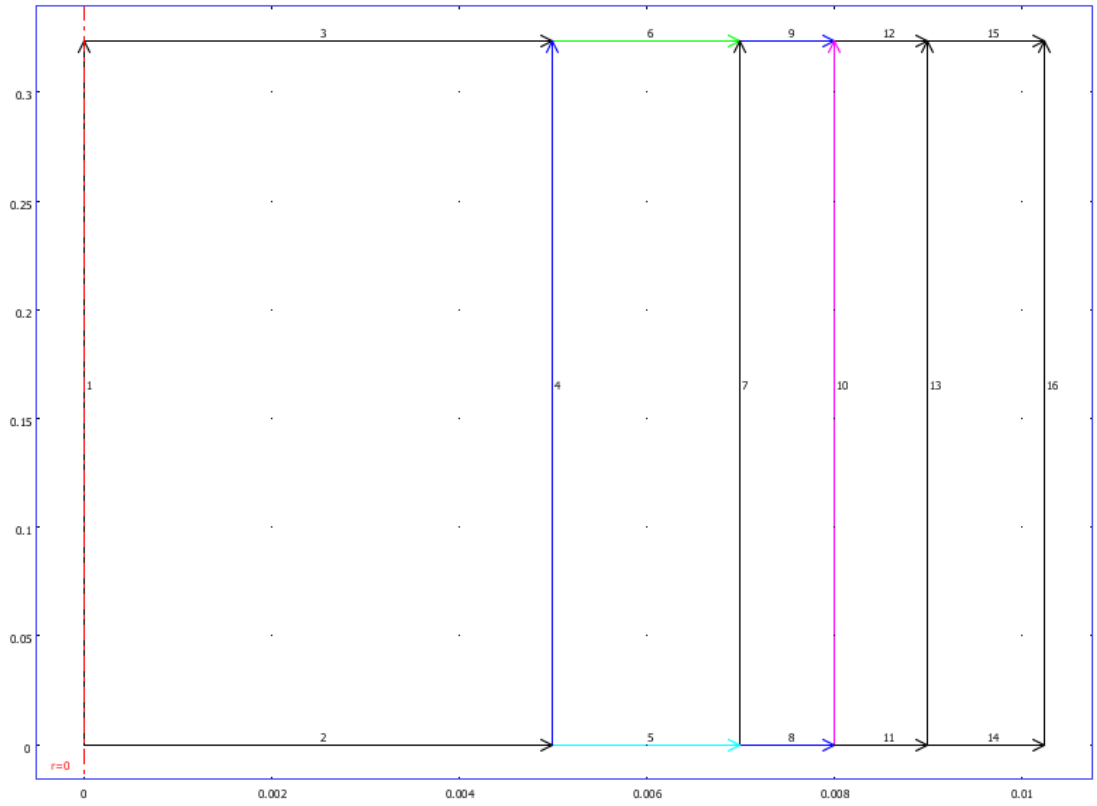
5.1. Geom1



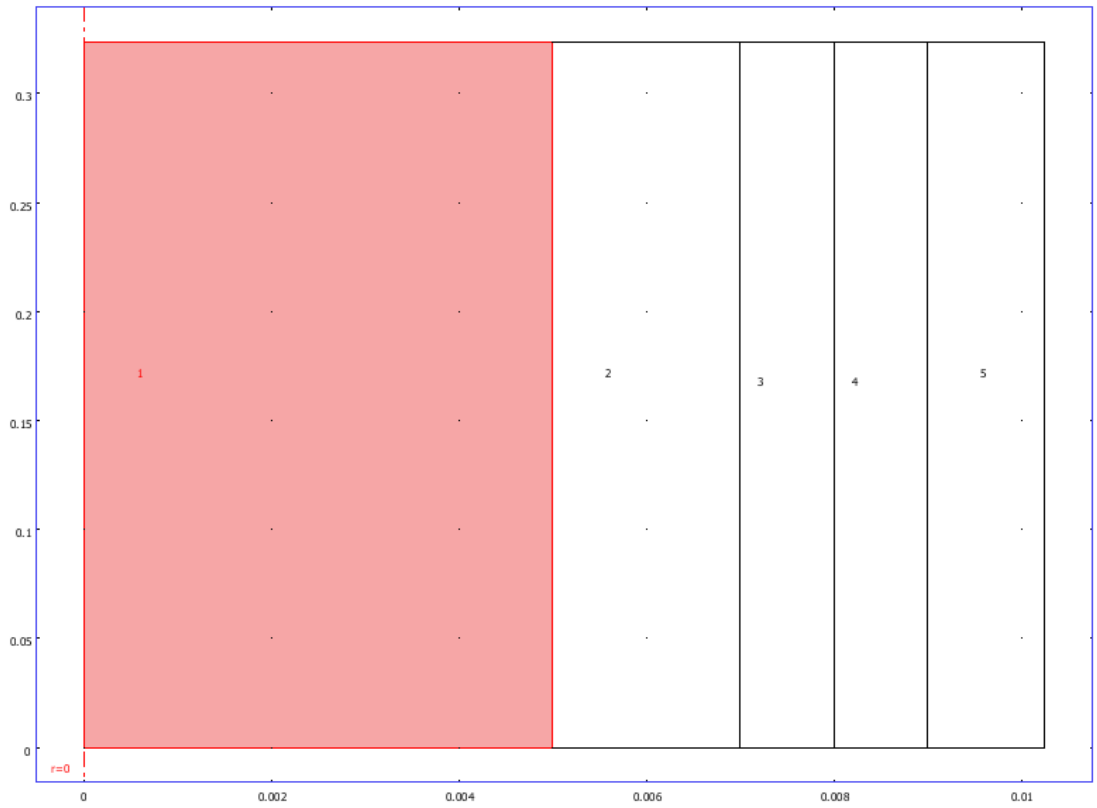
5.1.1. Point mode



5.1.2. Boundary mode



5.1.3. Subdomain mode



6. Geom1

Space dimensions: Axial symmetry (2D)

Independent variables: r, phi, z

6.1. Expressions

6.1.1. Subdomain Expressions

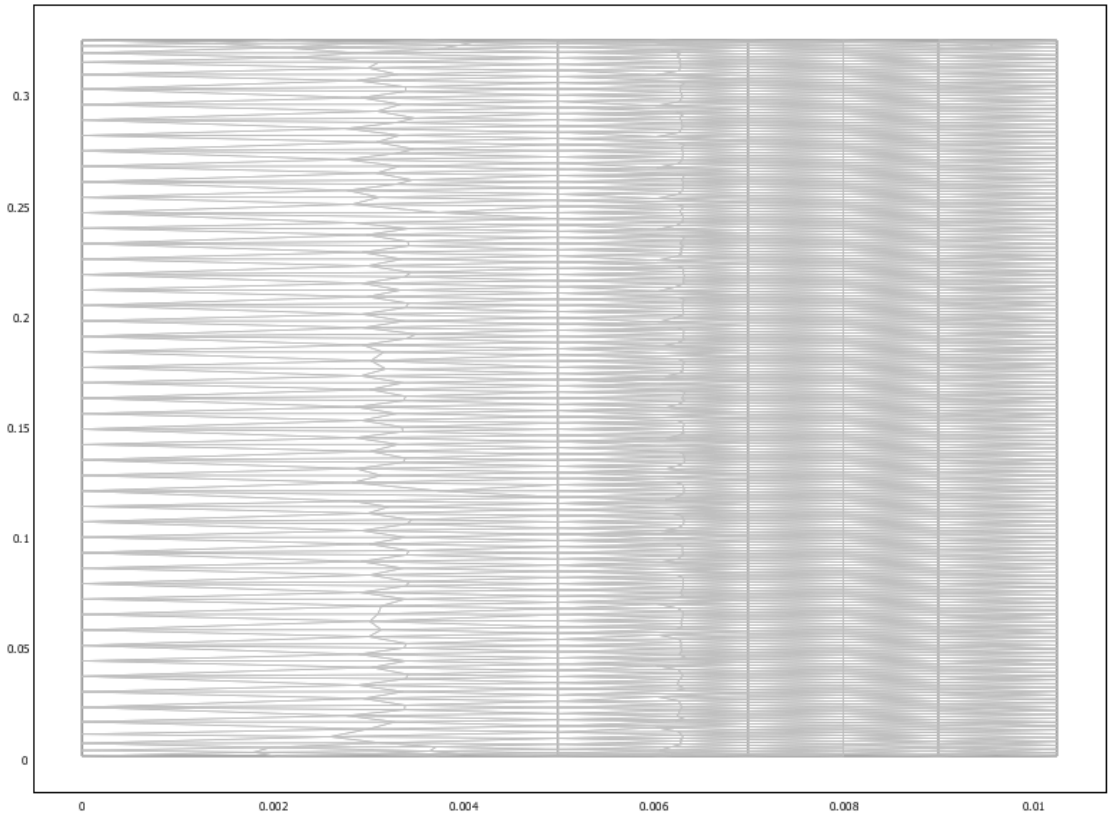
Subdomain		2	3	4	5
c_all	mol/m^3	cl	cl	cg	cg
mf_all	mol/m^3	x	x	y	y
IonS	mol/m^3	0.0005*(4*cco3+cna+coh)	0.0005*(4*cco3+cna+coh)		
logkb		11.895-2382/Temp+0.221*IonS-0.016*IonS^2	11.895-2382/Temp+0.221*IonS-0.016*IonS^2		
kb		0.001*exp(logkb)	0.001*exp(logkb)		
rate		kb*coh*cl	kb*coh*cl		

6.2. Mesh

6.2.1. Mesh Statistics

Number of degrees of freedom	13711

Number of mesh points	1427
Number of elements	2600
Triangular	2600
Quadrilateral	0
Number of boundary elements	1067
Number of vertex elements	12
Minimum element quality	0.644
Element area ratio	0.018



6.3. Application Mode: Convection and Diffusion (chcd)

Application mode type: Convection and Diffusion (Chemical Engineering Module)

Application mode name: chcd

6.3.1. Application Mode Properties

Property	**Value**
Default element type	Lagrange - Quadratic

Analysis type	Stationary
Equation form	Conservative
Equilibrium assumption	Off
Frame	Frame (ref)
Weak constraints	Off
Constraint type	Ideal

6.3.2. Variables

Dependent variables: cl

Shape functions: shlag(2,'cl')

Interior boundaries not active

6.3.3. Boundary Settings

Boundary		4, 8-9	5	6
Type		Insulation/Symmetry	Convective flux	Concentration
Inward flux (N)	$mol/(m^2 \cdot s)$	0	0	0
Concentration (c0)	mol/m^3	0	0	**cl0**

Boundary		10
Type		Flux
Inward flux (N)	$mol/(m^2 \cdot s)$	**M*(y-ye)**
Concentration (c0)	mol/m^3	0

6.3.4. Subdomain Settings

Subdomain		2	3
Diffusion coefficient (D)	m^2/s	**Dl**	**Deffl**
Diffusion coefficient (dtensor)	m^2/s	**{{Dl*10000,0;0,0}}**	**{{Deffl,0;0,0}}**
dtype		**aniso**	**aniso**
Reaction rate (R)	$mol/(m^3 \cdot s)$	**-1*rate**	**-1*rate**
z-velocity (v)	m/s	**vl**	0

6.4. Application Mode: Convection and Diffusion (chcd2)

Application mode type: Convection and Diffusion (Chemical Engineering Module)

Application mode name: chcd2

6.4.1. Application Mode Properties

Property	**Value**

Default element type	Lagrange - Quadratic
Analysis type	Stationary
Equation form	Conservative
Equilibrium assumption	Off
Frame	Frame (ref)
Weak constraints	Off
Constraint type	Ideal

6.4.2. Variables

Dependent variables: cg

Shape functions: shlag(2,'cg')

Interior boundaries not active

6.4.3. Boundary Settings

Boundary		10	11-12, 16	14
Type		Flux	Insulation/Symmetry	Concentration
Inward flux (N)	$mol/(m^2 \cdot s)$	**-M*(y-ye)**	0	0
Concentration (c0)	mol/m^3	0	0	**cg0**

Boundary		15
Type		Convective flux
Inward flux (N)	$mol/(m^2 \cdot s)$	0
Concentration (c0)	mol/m^3	0

6.4.4. Subdomain Settings

Subdomain		4	5
Diffusion coefficient (D)	m^2/s	**Deffg**	**Dg**
Diffusion coefficient (dtensor)	m^2/s	**{{Deffg,0;0,0}}**	**{{Dg,0;0,0}}**
dtype		**aniso**	**aniso**
z-velocity (v)	m/s	0	**vg**

6.5. Application Mode: Convection and Diffusion (chcd3)

Application mode type: Convection and Diffusion (Chemical Engineering Module)

Application mode name: chcd3

6.5.1. Application Mode Properties

Property	**Value**

Default element type	Lagrange - Quadratic
Analysis type	Stationary
Equation form	Conservative
Equilibrium assumption	Off
Frame	Frame (ref)
Weak constraints	Off
Constraint type	Ideal

6.5.2. Variables

Dependent variables: cco3, cna, coh

Shape functions: shlag(2,'cco3'), shlag(2,'cna'), shlag(2,'coh')

Interior boundaries not active

6.5.3. Boundary Settings

Boundary		4, 8-10	5	6
Type		Insulation/Symmetry	Convective flux	Concentration
Concentration (c0)	mol/m^3	{0;0;0}	{0;0;0}	**{Cco30;Cna0;Coh0}**

6.5.4. Subdomain Settings

Subdomain		2	3
Diffusion coefficient (dtensor)	m^2/s	**{{1,0;0,1};{Dl*10000,0;0,1};{Dl*10000*2,0;0,1}}**	**{{Deffl,0;0,1};{1,0;0,1};{1,0;0,1}}**
dtype		**{aniso;aniso;aniso}**	**{aniso;aniso;aniso}**
Reaction rate (R)	$mol/(m^3 \cdot s)$	**{rate;0;-2*rate}**	**{rate;0;-2*rate}**
z-velocity (v)	m/s	**{vl;vl;vl}**	{0;0;0}

7. Solver Settings

Solve using a script: off

Analysis type	Stationary
Auto select solver	On
Solver	Stationary

Solution form	Automatic
Symmetric	auto
Adaptive mesh refinement	Off
Optimization/Sensitivity	Off
Plot while solving	Off

7.1. Direct (UMFPACK)

Solver type: Linear system solver

Parameter	**Value**
Pivot threshold	0.1
Memory allocation factor	0.7

7.2. Stationary

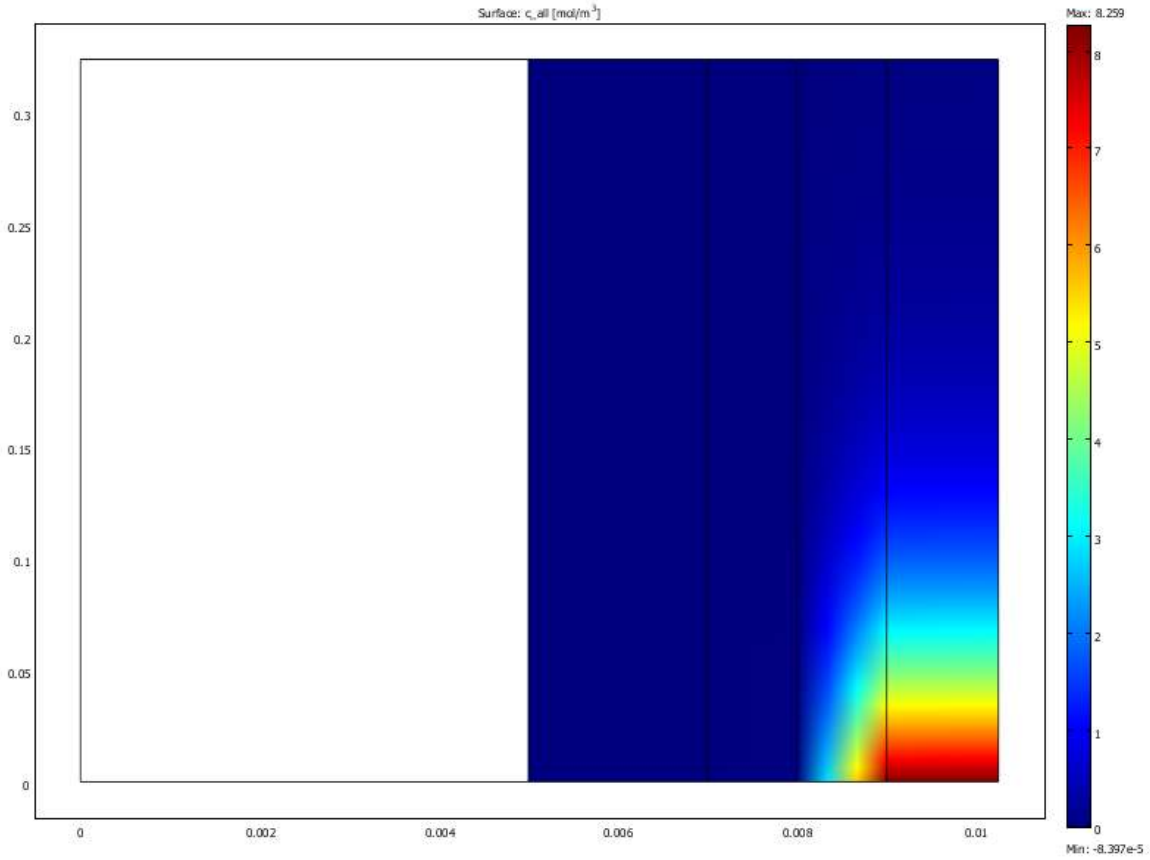
Parameter	**Value**
Linearity	Automatic
Relative tolerance	1.0E-6
Maximum number of iterations	25
Manual tuning of damping parameters	Off
Highly nonlinear problem	Off
Initial damping factor	1.0
Minimum damping factor	1.0E-4
Restriction for step size update	10.0

7.3. Advanced

Parameter	**Value**
Constraint handling method	Elimination
Null-space function	Automatic
Automatic assembly block size	On
Assembly block size	5000
Use Hermitian transpose of constraint matrix and in symmetry detection	Off
Use complex functions with real input	Off
Stop if error due to undefined operation	On
Store solution on file	Off
Type of scaling	Automatic
Manual scaling	
Row equilibration	On
Manual control of reassembly	Off

Load constant	On
Constraint constant	On
Mass constant	On
Damping (mass) constant	On
Jacobian constant	On
Constraint Jacobian constant	On

8. Postprocessing



9. Variables

9.1. Boundary

9.1.1. Boundary 1-3

Name	Description	Unit	Expression
ndflux_cl_chcd	Normal diffusive flux, cl	mol/(m^2*s)	
ncflux_cl_chcd	Normal convective flux, cl	mol/(m^2*s)	
ntflux_cl_chcd	Normal total flux, cl	mol/(m^2*s)	
ndflux_cg_chcd2	Normal diffusive flux, cg	mol/(m^2*s)	
ncflux_cg_chcd2	Normal convective flux, cg	mol/(m^2*s)	
ntflux_cg_chcd2	Normal total flux, cg	mol/(m^2*s)	
ndflux_cco3_chcd3	Normal diffusive flux, cco3	mol/(m^2*s)	

ncflux_cco3_chcd3	Normal convective flux, cco3	mol/(m^2*s)	
ntflux_cco3_chcd3	Normal total flux, cco3	mol/(m^2*s)	
ndflux_cna_chcd3	Normal diffusive flux, cna	mol/(m^2*s)	
ncflux_cna_chcd3	Normal convective flux, cna	mol/(m^2*s)	
ntflux_cna_chcd3	Normal total flux, cna	mol/(m^2*s)	
ndflux_coh_chcd3	Normal diffusive flux, coh	mol/(m^2*s)	
ncflux_coh_chcd3	Normal convective flux, coh	mol/(m^2*s)	
ntflux_coh_chcd3	Normal total flux, coh	mol/(m^2*s)	

9.1.2. Boundary 4-9

Name	Description	Unit	Expression
ndflux_cl_chcd	Normal diffusive flux, cl	mol/(m^2*s)	nr_chcd * dflux_cl_r_chcd+nz_chcd * dflux_cl_z_chcd
ncflux_cl_chcd	Normal convective flux, cl	mol/(m^2*s)	nr_chcd * cflux_cl_r_chcd+nz_chcd * cflux_cl_z_chcd
ntflux_cl_chcd	Normal total flux, cl	mol/(m^2*s)	nr_chcd * tflux_cl_r_chcd+nz_chcd * tflux_cl_z_chcd
ndflux_cg_chcd2	Normal diffusive flux, cg	mol/(m^2*s)	
ncflux_cg_chcd2	Normal convective flux, cg	mol/(m^2*s)	
ntflux_cg_chcd2	Normal total flux, cg	mol/(m^2*s)	
ndflux_cco3_chcd3	Normal diffusive flux, cco3	mol/(m^2*s)	nr_chcd3 * dflux_cco3_r_chcd3+nz_chcd3 * dflux_cco3_z_chcd3
ncflux_cco3_chcd3	Normal convective flux, cco3	mol/(m^2*s)	nr_chcd3 * cflux_cco3_r_chcd3+nz_chcd3 * cflux_cco3_z_chcd3
ntflux_cco3_chcd3	Normal total flux, cco3	mol/(m^2*s)	nr_chcd3 * tflux_cco3_r_chcd3+nz_chcd3 * tflux_cco3_z_chcd3
ndflux_cna_chcd3	Normal diffusive flux, cna	mol/(m^2*s)	nr_chcd3 * dflux_cna_r_chcd3+nz_chcd3 * dflux_cna_z_chcd3
ncflux_cna_chcd3	Normal convective	mol/(m^2*s)	nr_chcd3 * cflux_cna_r_chcd3+nz_chcd3 *

	flux, cna		cflux_cna_z_chcd3
ntflux_cna_chcd3	Normal total flux, cna	mol/(m^2*s)	nr_chcd3 * tflux_cna_r_chcd3+nz_chcd3 * tflux_cna_z_chcd3
ndflux_coh_chcd3	Normal diffusive flux, coh	mol/(m^2*s)	nr_chcd3 * dflux_coh_r_chcd3+nz_chcd3 * dflux_coh_z_chcd3
ncflux_coh_chcd3	Normal convective flux, coh	mol/(m^2*s)	nr_chcd3 * cflux_coh_r_chcd3+nz_chcd3 * cflux_coh_z_chcd3
ntflux_coh_chcd3	Normal total flux, coh	mol/(m^2*s)	nr_chcd3 * tflux_coh_r_chcd3+nz_chcd3 * tflux_coh_z_chcd3

9.1.3. Boundary 10

Name	**Description**	**Unit**	**Expression**
ndflux_cl_chcd	Normal diffusive flux, cl	mol/(m^2*s)	nr_chcd * dflux_cl_r_chcd+nz_chcd * dflux_cl_z_chcd
ncflux_cl_chcd	Normal convective flux, cl	mol/(m^2*s)	nr_chcd * cflux_cl_r_chcd+nz_chcd * cflux_cl_z_chcd
ntflux_cl_chcd	Normal total flux, cl	mol/(m^2*s)	nr_chcd * tflux_cl_r_chcd+nz_chcd * tflux_cl_z_chcd
ndflux_cg_chcd2	Normal diffusive flux, cg	mol/(m^2*s)	nr_chcd2 * dflux_cg_r_chcd2+nz_chcd2 * dflux_cg_z_chcd2
ncflux_cg_chcd2	Normal convective flux, cg	mol/(m^2*s)	nr_chcd2 * cflux_cg_r_chcd2+nz_chcd2 * cflux_cg_z_chcd2
ntflux_cg_chcd2	Normal total flux, cg	mol/(m^2*s)	nr_chcd2 * tflux_cg_r_chcd2+nz_chcd2 * tflux_cg_z_chcd2
ndflux_cco3_chcd3	Normal diffusive flux, cco3	mol/(m^2*s)	nr_chcd3 * dflux_cco3_r_chcd3+nz_chcd3 * dflux_cco3_z_chcd3
ncflux_cco3_chcd3	Normal convective flux, cco3	mol/(m^2*s)	nr_chcd3 * cflux_cco3_r_chcd3+nz_chcd3 * cflux_cco3_z_chcd3
ntflux_cco3_chcd3	Normal total flux, cco3	mol/(m^2*s)	nr_chcd3 * tflux_cco3_r_chcd3+nz_chcd3 * tflux_cco3_z_chcd3

ndflux_cna_chcd3	Normal diffusive flux, cna	mol/(m^2*s)	nr_chcd3 * dflux_cna_r_chcd3+nz_chcd3 * dflux_cna_z_chcd3
ncflux_cna_chcd3	Normal convective flux, cna	mol/(m^2*s)	nr_chcd3 * cflux_cna_r_chcd3+nz_chcd3 * cflux_cna_z_chcd3
ntflux_cna_chcd3	Normal total flux, cna	mol/(m^2*s)	nr_chcd3 * tflux_cna_r_chcd3+nz_chcd3 * tflux_cna_z_chcd3
ndflux_coh_chcd3	Normal diffusive flux, coh	mol/(m^2*s)	nr_chcd3 * dflux_coh_r_chcd3+nz_chcd3 * dflux_coh_z_chcd3
ncflux_coh_chcd3	Normal convective flux, coh	mol/(m^2*s)	nr_chcd3 * cflux_coh_r_chcd3+nz_chcd3 * cflux_coh_z_chcd3
ntflux_coh_chcd3	Normal total flux, coh	mol/(m^2*s)	nr_chcd3 * tflux_coh_r_chcd3+nz_chcd3 * tflux_coh_z_chcd3

9.1.4. Boundary 11-16

Name	Description	Unit	Expression
ndflux_cl_chcd	Normal diffusive flux, cl	mol/(m^2*s)	
ncflux_cl_chcd	Normal convective flux, cl	mol/(m^2*s)	
ntflux_cl_chcd	Normal total flux, cl	mol/(m^2*s)	
ndflux_cg_chcd2	Normal diffusive flux, cg	mol/(m^2*s)	nr_chcd2 * dflux_cg_r_chcd2+nz_chcd2 * dflux_cg_z_chcd2
ncflux_cg_chcd2	Normal convective flux, cg	mol/(m^2*s)	nr_chcd2 * cflux_cg_r_chcd2+nz_chcd2 * cflux_cg_z_chcd2
ntflux_cg_chcd2	Normal total flux, cg	mol/(m^2*s)	nr_chcd2 * tflux_cg_r_chcd2+nz_chcd2 * tflux_cg_z_chcd2
ndflux_cco3_chcd3	Normal diffusive flux, cco3	mol/(m^2*s)	
ncflux_cco3_chcd3	Normal convective flux,	mol/(m^2*s)	

	cco3		
ntflux_cco3_chcd3	Normal total flux, cco3	mol/(m^2*s)	
ndflux_cna_chcd3	Normal diffusive flux, cna	mol/(m^2*s)	
ncflux_cna_chcd3	Normal convective flux, cna	mol/(m^2*s)	
ntflux_cna_chcd3	Normal total flux, cna	mol/(m^2*s)	
ndflux_coh_chcd3	Normal diffusive flux, coh	mol/(m^2*s)	
ncflux_coh_chcd3	Normal convective flux, coh	mol/(m^2*s)	
ntflux_coh_chcd3	Normal total flux, coh	mol/(m^2*s)	

9.2. Subdomain

9.2.1. Subdomain 1

Name	Description	Unit	Expression
grad_cl_r_chcd	Concentration gradient, cl, r component	mol/m^4	
dflux_cl_r_chcd	Diffusive flux, cl, r component	mol/(m^2*s)	
cflux_cl_r_chcd	Convective flux, cl, r component	mol/(m^2*s)	
tflux_cl_r_chcd	Total flux, cl, r component	mol/(m^2*s)	
grad_cl_z_chcd	Concentration gradient, cl, z component	mol/m^4	
dflux_cl_z_chcd	Diffusive flux, cl, z component	mol/(m^2*s)	
cflux_cl_z_chcd	Convective flux, cl, z component	mol/(m^2*s)	
tflux_cl_z_chcd	Total flux, cl, z component	mol/(m^2*s)	
beta_cl_r_chcd	Convective field, cl, r component	m^2/s	
beta_cl_z_chcd	Convective field, cl, z component	m^2/s	
grad_cl_chcd	Concentration gradient, cl	mol/m^4	
dflux_cl_chcd	Diffusive flux, cl	mol/(m^2*s)	
cflux_cl_chcd	Convective flux, cl	mol/(m^2*s)	
tflux_cl_chcd	Total flux, cl	mol/(m^2*s)	
cellPe_cl_chcd	Cell Peclet number, cl	1	
Dm_cl_chcd	Mean diffusion coefficient, cl	m^3/s	

res_cl_chcd	Equation residual for cl	mol/(m^2*s)	
res_sc_cl_chcd	Shock capturing residual for cl	mol/(m^2*s)	
da_cl_chcd	Total time scale factor, cl	m	
grad_cg_r_chcd2	Concentration gradient, cg, r component	mol/m^4	
dflux_cg_r_chcd2	Diffusive flux, cg, r component	mol/(m^2*s)	
cflux_cg_r_chcd2	Convective flux, cg, r component	mol/(m^2*s)	
tflux_cg_r_chcd2	Total flux, cg, r component	mol/(m^2*s)	
grad_cg_z_chcd2	Concentration gradient, cg, z component	mol/m^4	
dflux_cg_z_chcd2	Diffusive flux, cg, z component	mol/(m^2*s)	
cflux_cg_z_chcd2	Convective flux, cg, z component	mol/(m^2*s)	
tflux_cg_z_chcd2	Total flux, cg, z component	mol/(m^2*s)	
beta_cg_r_chcd2	Convective field, cg, r component	m^2/s	
beta_cg_z_chcd2	Convective field, cg, z component	m^2/s	
grad_cg_chcd2	Concentration gradient, cg	mol/m^4	
dflux_cg_chcd2	Diffusive flux, cg	mol/(m^2*s)	
cflux_cg_chcd2	Convective flux, cg	mol/(m^2*s)	
tflux_cg_chcd2	Total flux, cg	mol/(m^2*s)	
cellPe_cg_chcd2	Cell Peclet number, cg	1	
Dm_cg_chcd2	Mean diffusion coefficient, cg	m^3/s	
res_cg_chcd2	Equation residual for cg	mol/(m^2*s)	
res_sc_cg_chcd2	Shock capturing residual for cg	mol/(m^2*s)	
da_cg_chcd2	Total time scale factor, cg	m	
grad_cco3_r_chcd3	Concentration gradient, cco3, r component	mol/m^4	
dflux_cco3_r_chcd3	Diffusive flux, cco3, r component	mol/(m^2*s)	
cflux_cco3_r_chcd3	Convective flux, cco3, r component	mol/(m^2*s)	
tflux_cco3_r_chcd3	Total flux, cco3, r component	mol/(m^2*s)	
grad_cco3_z_chcd3	Concentration gradient, cco3, z component	mol/m^4	
dflux_cco3_z_chcd3	Diffusive flux, cco3, z component	mol/(m^2*s)	
cflux_cco3_z_chcd3	Convective flux, cco3, z component	mol/(m^2*s)	
tflux_cco3_z_chcd3	Total flux, cco3, z component	mol/(m^2*s)	
beta_cco3_r_chcd3	Convective field, cco3, r component	m^2/s	
beta_cco3_z_chcd3	Convective field, cco3, z component	m^2/s	
grad_cco3_chcd3	Concentration gradient, cco3	mol/m^4	

dflux_cco3_chcd3	Diffusive flux, cco3	mol/(m^2*s)	
cflux_cco3_chcd3	Convective flux, cco3	mol/(m^2*s)	
tflux_cco3_chcd3	Total flux, cco3	mol/(m^2*s)	
cellPe_cco3_chcd3	Cell Peclet number, cco3	1	
Dm_cco3_chcd3	Mean diffusion coefficient, cco3	m^3/s	
res_cco3_chcd3	Equation residual for cco3	mol/(m^2*s)	
res_sc_cco3_chcd3	Shock capturing residual for cco3	mol/(m^2*s)	
da_cco3_chcd3	Total time scale factor, cco3	m	
grad_cna_r_chcd3	Concentration gradient, cna, r component	mol/m^4	
dflux_cna_r_chcd3	Diffusive flux, cna, r component	mol/(m^2*s)	
cflux_cna_r_chcd3	Convective flux, cna, r component	mol/(m^2*s)	
tflux_cna_r_chcd3	Total flux, cna, r component	mol/(m^2*s)	
grad_cna_z_chcd3	Concentration gradient, cna, z component	mol/m^4	
dflux_cna_z_chcd3	Diffusive flux, cna, z component	mol/(m^2*s)	
cflux_cna_z_chcd3	Convective flux, cna, z component	mol/(m^2*s)	
tflux_cna_z_chcd3	Total flux, cna, z component	mol/(m^2*s)	
beta_cna_r_chcd3	Convective field, cna, r component	m^2/s	
beta_cna_z_chcd3	Convective field, cna, z component	m^2/s	
grad_cna_chcd3	Concentration gradient, cna	mol/m^4	
dflux_cna_chcd3	Diffusive flux, cna	mol/(m^2*s)	
cflux_cna_chcd3	Convective flux, cna	mol/(m^2*s)	
tflux_cna_chcd3	Total flux, cna	mol/(m^2*s)	
cellPe_cna_chcd3	Cell Peclet number, cna	1	
Dm_cna_chcd3	Mean diffusion coefficient, cna	m^3/s	
res_cna_chcd3	Equation residual for cna	mol/(m^2*s)	
res_sc_cna_chcd3	Shock capturing residual for cna	mol/(m^2*s)	
da_cna_chcd3	Total time scale factor, cna	m	
grad_coh_r_chcd3	Concentration gradient, coh, r component	mol/m^4	
dflux_coh_r_chcd3	Diffusive flux, coh, r component	mol/(m^2*s)	
cflux_coh_r_chcd3	Convective flux, coh, r component	mol/(m^2*s)	
tflux_coh_r_chcd3	Total flux, coh, r component	mol/(m^2*s)	
grad_coh_z_chcd3	Concentration gradient, coh, z component	mol/m^4	
dflux_coh_z_chcd3	Diffusive flux, coh, z component	mol/(m^2*s)	

cflux_coh_z_chcd3	Convective flux, coh, z component	mol/(m^2*s)	
tflux_coh_z_chcd3	Total flux, coh, z component	mol/(m^2*s)	
beta_coh_r_chcd3	Convective field, coh, r component	m^2/s	
beta_coh_z_chcd3	Convective field, coh, z component	m^2/s	
grad_coh_chcd3	Concentration gradient, coh	mol/m^4	
dflux_coh_chcd3	Diffusive flux, coh	mol/(m^2*s)	
cflux_coh_chcd3	Convective flux, coh	mol/(m^2*s)	
tflux_coh_chcd3	Total flux, coh	mol/(m^2*s)	
cellPe_coh_chcd3	Cell Peclet number, coh	1	
Dm_coh_chcd3	Mean diffusion coefficient, coh	m^3/s	
res_coh_chcd3	Equation residual for coh	mol/(m^2*s)	
res_sc_coh_chcd3	Shock capturing residual for coh	mol/(m^2*s)	
da_coh_chcd3	Total time scale factor, coh	m	

9.2.2. Subdomain 2-3

Name	Description	Unit	Expression
grad_cl_r_chcd	Concentration gradient, cl, r component	mol/m^4	clr
dflux_cl_r_chcd	Diffusive flux, cl, r component	mol/(m^2*s)	-Drr_cl_chcd * clr-Drz_cl_chcd * clz
cflux_cl_r_chcd	Convective flux, cl, r component	mol/(m^2*s)	cl * u_cl_chcd
tflux_cl_r_chcd	Total flux, cl, r component	mol/(m^2*s)	dflux_cl_r_chcd+cflux_cl_r_chcd
grad_cl_z_chcd	Concentration gradient, cl, z componen	mol/m^4	clz

	t		
dflux_cl_z_chcd	Diffusive flux, cl, z component	mol/(m^2*s)	-Dzr_cl_chcd * clr-Dzz_cl_chcd * clz
cflux_cl_z_chcd	Convective flux, cl, z component	mol/(m^2*s)	cl * v_cl_chcd
tflux_cl_z_chcd	Total flux, cl, z component	mol/(m^2*s)	dflux_cl_z_chcd+cflux_cl_z_chcd
beta_cl_r_chcd	Convective field, cl, r component	m^2/s	r * u_cl_chcd
beta_cl_z_chcd	Convective field, cl, z component	m^2/s	r * v_cl_chcd
grad_cl_chcd	Concentration gradient, cl	mol/m^4	sqrt(grad_cl_r_chcd^2+grad_cl_z_chcd^2)
dflux_cl_chcd	Diffusive flux, cl	mol/(m^2*s)	sqrt(dflux_cl_r_chcd^2+dflux_cl_z_chcd^2)
cflux_cl_chcd	Convective flux, cl	mol/(m^2*s)	sqrt(cflux_cl_r_chcd^2+cflux_cl_z_chcd^2)
tflux_cl_chcd	Total flux, cl	mol/(m^2*s)	sqrt(tflux_cl_r_chcd^2+tflux_cl_z_chcd^2)
cellPe_cl_chcd	Cell Peclet number, cl	1	h * sqrt(beta_cl_r_chcd^2+beta_cl_z_chcd^2)/Dm_cl_chcd
Dm_cl_chcd	Mean diffusion coefficient, cl	m^3/s	r * (Drr_cl_chcd * u_cl_chcd^2+Drz_cl_chcd * u_cl_chcd * v_cl_chcd+Dzr_cl_chcd * v_cl_chcd * u_cl_chcd+Dzz_cl_chcd * v_cl_chcd^2)/(u_cl_chcd^2+v_cl_chcd^2+eps)

res_cl_chcd	Equation residual for cl	mol/(m^2*s)	r * (-Drr_cl_chcd * clrr-Drz_cl_chcd * clrz+clr * u_cl_chcd-Dzr_cl_chcd * clzr-Dzz_cl_chcd * clzz+clz * v_cl_chcd-R_cl_chcd)
res_sc_cl_chcd	Shock capturing residual for cl	mol/(m^2*s)	r * (clr * u_cl_chcd+clz * v_cl_chcd-R_cl_chcd)
da_cl_chcd	Total time scale factor, cl	m	r * Dts_cl_chcd
grad_cg_r_chcd2	Concentration gradient, cg, r component	mol/m^4	
dflux_cg_r_chcd2	Diffusive flux, cg, r component	mol/(m^2*s)	
cflux_cg_r_chcd2	Convective flux, cg, r component	mol/(m^2*s)	
tflux_cg_r_chcd2	Total flux, cg, r component	mol/(m^2*s)	
grad_cg_z_chcd2	Concentration gradient, cg, z component	mol/m^4	
dflux_cg_z_chcd2	Diffusive flux, cg, z component	mol/(m^2*s)	
cflux_cg_z_chcd2	Convective flux, cg, z componen	mol/(m^2*s)	

	t		
tflux_cg_z_chcd2	Total flux, cg, z component	mol/(m^2*s)	
beta_cg_r_chcd2	Convective field, cg, r component	m^2/s	
beta_cg_z_chcd2	Convective field, cg, z component	m^2/s	
grad_cg_chcd2	Concentration gradient, cg	mol/m^4	
dflux_cg_chcd2	Diffusive flux, cg	mol/(m^2*s)	
cflux_cg_chcd2	Convective flux, cg	mol/(m^2*s)	
tflux_cg_chcd2	Total flux, cg	mol/(m^2*s)	
cellPe_cg_chcd2	Cell Peclet number, cg	1	
Dm_cg_chcd2	Mean diffusion coefficient, cg	m^3/s	
res_cg_chcd2	Equation residual for cg	mol/(m^2*s)	
res_sc_cg_chcd2	Shock capturing residual for cg	mol/(m^2*s)	
da_cg_chcd2	Total time scale	m	

	factor, cg		
grad_cco3_r_chcd3	Concentration gradient, cco3, r component	mol/m^4	cco3r
dflux_cco3_r_chcd3	Diffusive flux, cco3, r component	mol/(m^2*s)	-Drr_cco3_chcd3 * cco3r-Drz_cco3_chcd3 * cco3z
cflux_cco3_r_chcd3	Convective flux, cco3, r component	mol/(m^2*s)	cco3 * u_cco3_chcd3
tflux_cco3_r_chcd3	Total flux, cco3, r component	mol/(m^2*s)	dflux_cco3_r_chcd3+cflux_cco3_r_chcd3
grad_cco3_z_chcd3	Concentration gradient, cco3, z component	mol/m^4	cco3z
dflux_cco3_z_chcd3	Diffusive flux, cco3, z component	mol/(m^2*s)	-Dzr_cco3_chcd3 * cco3r-Dzz_cco3_chcd3 * cco3z
cflux_cco3_z_chcd3	Convective flux, cco3, z component	mol/(m^2*s)	cco3 * v_cco3_chcd3
tflux_cco3_z_chcd3	Total flux, cco3, z component	mol/(m^2*s)	dflux_cco3_z_chcd3+cflux_cco3_z_chcd3
beta_cco3_r_chcd3	Convective field,	m^2/s	r * u_cco3_chcd3

	cco3, r component		
beta_cco3_z_chcd3	Convective field, cco3, z component	m^2/s	r * v_cco3_chcd3
grad_cco3_chcd3	Concentration gradient, cco3	mol/m^4	sqrt(grad_cco3_r_chcd3^2+grad_cco3_z_chcd3^2)
dflux_cco3_chcd3	Diffusive flux, cco3	mol/(m^2*s)	sqrt(dflux_cco3_r_chcd3^2+dflux_cco3_z_chcd3^2)
cflux_cco3_chcd3	Convective flux, cco3	mol/(m^2*s)	sqrt(cflux_cco3_r_chcd3^2+cflux_cco3_z_chcd3^2)
tflux_cco3_chcd3	Total flux, cco3	mol/(m^2*s)	sqrt(tflux_cco3_r_chcd3^2+tflux_cco3_z_chcd3^2)
cellPe_cco3_chcd3	Cell Peclet number, cco3	1	h * sqrt(beta_cco3_r_chcd3^2+beta_cco3_z_chcd3^2) /Dm_cco3_chcd3
Dm_cco3_chcd3	Mean diffusion coefficient, cco3	m^3/s	r * (Drr_cco3_chcd3 * u_cco3_chcd3^2+Drz_cco3_chcd3 * u_cco3_chcd3 * v_cco3_chcd3+Dzr_cco3_chcd3 * v_cco3_chcd3 * u_cco3_chcd3+Dzz_cco3_chcd3 * v_cco3_chcd3^2)/(u_cco3_chcd3^2+v_cco3_chcd3^2+eps)
res_cco3_chcd3	Equation residual for cco3	mol/(m^2*s)	r * (-Drr_cco3_chcd3 * cco3rr-Drz_cco3_chcd3 * cco3rz+cco3r * u_cco3_chcd3-Dzr_cco3_chcd3 * cco3zr-Dzz_cco3_chcd3 * cco3zz+cco3z * v_cco3_chcd3-R_cco3_chcd3)
res_sc_cco3_chcd3	Shock capturing residual for cco3	mol/(m^2*s)	r * (cco3r * u_cco3_chcd3+cco3z * v_cco3_chcd3-R_cco3_chcd3)
da_cco3_chcd3	Total time scale factor, cco3	m	r * Dts_cco3_chcd3

grad_cna_r_chcd3	Concentration gradient, cna, r component	mol/m^4	cnar
dflux_cna_r_chcd3	Diffusive flux, cna, r component	mol/(m^2*s)	-Drr_cna_chcd3 * cnar-Drz_cna_chcd3 * cnaz
cflux_cna_r_chcd3	Convective flux, cna, r component	mol/(m^2*s)	cna * u_cna_chcd3
tflux_cna_r_chcd3	Total flux, cna, r component	mol/(m^2*s)	dflux_cna_r_chcd3+cflux_cna_r_chcd3
grad_cna_z_chcd3	Concentration gradient, cna, z component	mol/m^4	cnaz
dflux_cna_z_chcd3	Diffusive flux, cna, z component	mol/(m^2*s)	-Dzr_cna_chcd3 * cnar-Dzz_cna_chcd3 * cnaz
cflux_cna_z_chcd3	Convective flux, cna, z component	mol/(m^2*s)	cna * v_cna_chcd3
tflux_cna_z_chcd3	Total flux, cna, z component	mol/(m^2*s)	dflux_cna_z_chcd3+cflux_cna_z_chcd3
beta_cna_r_chcd3	Convective field, cna, r	m^2/s	r * u_cna_chcd3

	component		
beta_cna_z_chcd3	Convective field, cna, z component	m^2/s	r * v_cna_chcd3
grad_cna_chcd3	Concentration gradient, cna	mol/m^4	sqrt(grad_cna_r_chcd3^2+grad_cna_z_chcd3^2)
dflux_cna_chcd3	Diffusive flux, cna	mol/(m^2*s)	sqrt(dflux_cna_r_chcd3^2+dflux_cna_z_chcd3^2)
cflux_cna_chcd3	Convective flux, cna	mol/(m^2*s)	sqrt(cflux_cna_r_chcd3^2+cflux_cna_z_chcd3^2)
tflux_cna_chcd3	Total flux, cna	mol/(m^2*s)	sqrt(tflux_cna_r_chcd3^2+tflux_cna_z_chcd3^2)
cellPe_cna_chcd3	Cell Peclet number, cna	1	h * sqrt(beta_cna_r_chcd3^2+beta_cna_z_chcd3^2)/Dm_cna_chcd3
Dm_cna_chcd3	Mean diffusion coefficient, cna	m^3/s	r * (Drr_cna_chcd3 * u_cna_chcd3^2+Drz_cna_chcd3 * u_cna_chcd3 * v_cna_chcd3+Dzr_cna_chcd3 * v_cna_chcd3 * u_cna_chcd3+Dzz_cna_chcd3 * v_cna_chcd3^2)/(u_cna_chcd3^2+v_cna_chcd3^2+eps)
res_cna_chcd3	Equation residual for cna	mol/(m^2*s)	r * (-Drr_cna_chcd3 * cnarr-Drz_cna_chcd3 * cnarz+cnar * u_cna_chcd3-Dzr_cna_chcd3 * cnazr-Dzz_cna_chcd3 * cnazz+cnaz * v_cna_chcd3-R_cna_chcd3)
res_sc_cna_chcd3	Shock capturing residual for cna	mol/(m^2*s)	r * (cnar * u_cna_chcd3+cnaz * v_cna_chcd3-R_cna_chcd3)
da_cna_chcd3	Total time scale factor, cna	m	r * Dts_cna_chcd3
grad_coh_r_chcd3	Concentration gradient, coh, r	mol/m^4	cohr

	component		
dflux_coh_r_chcd3	Diffusive flux, coh, r component	mol/(m^2*s)	-Drr_coh_chcd3 * cohr-Drz_coh_chcd3 * cohz
cflux_coh_r_chcd3	Convective flux, coh, r component	mol/(m^2*s)	coh * u_coh_chcd3
tflux_coh_r_chcd3	Total flux, coh, r component	mol/(m^2*s)	dflux_coh_r_chcd3+cflux_coh_r_chcd3
grad_coh_z_chcd3	Concentration gradient, coh, z component	mol/m^4	cohz
dflux_coh_z_chcd3	Diffusive flux, coh, z component	mol/(m^2*s)	-Dzr_coh_chcd3 * cohr-Dzz_coh_chcd3 * cohz
cflux_coh_z_chcd3	Convective flux, coh, z component	mol/(m^2*s)	coh * v_coh_chcd3
tflux_coh_z_chcd3	Total flux, coh, z component	mol/(m^2*s)	dflux_coh_z_chcd3+cflux_coh_z_chcd3
beta_coh_r_chcd3	Convective field, coh, r component	m^2/s	r * u_coh_chcd3
beta_coh_z_chcd3	Convective field,	m^2/s	r * v_coh_chcd3

	coh, z component		
grad_coh_chcd3	Concentration gradient, coh	mol/m^4	sqrt(grad_coh_r_chcd3^2+grad_coh_z_chcd3^2)
dflux_coh_chcd3	Diffusive flux, coh	mol/(m^2*s)	sqrt(dflux_coh_r_chcd3^2+dflux_coh_z_chcd3^2)
cflux_coh_chcd3	Convective flux, coh	mol/(m^2*s)	sqrt(cflux_coh_r_chcd3^2+cflux_coh_z_chcd3^2)
tflux_coh_chcd3	Total flux, coh	mol/(m^2*s)	sqrt(tflux_coh_r_chcd3^2+tflux_coh_z_chcd3^2)
cellPe_coh_chcd3	Cell Peclet number, coh	1	h * sqrt(beta_coh_r_chcd3^2+beta_coh_z_chcd3^2)/Dm_coh_chcd3
Dm_coh_chcd3	Mean diffusion coefficient, coh	m^3/s	r * (Drr_coh_chcd3 * u_coh_chcd3^2+Drz_coh_chcd3 * u_coh_chcd3 * v_coh_chcd3+Dzr_coh_chcd3 * v_coh_chcd3 * u_coh_chcd3+Dzz_coh_chcd3 * v_coh_chcd3^2)/(u_coh_chcd3^2+v_coh_chcd3^2+eps)
res_coh_chcd3	Equation residual for coh	mol/(m^2*s)	r * (-Drr_coh_chcd3 * cohrr-Drz_coh_chcd3 * cohrz+cohr * u_coh_chcd3-Dzr_coh_chcd3 * cohzr-Dzz_coh_chcd3 * cohzz+cohz * v_coh_chcd3-R_coh_chcd3)
res_sc_coh_chcd3	Shock capturing residual for coh	mol/(m^2*s)	r * (cohr * u_coh_chcd3+cohz * v_coh_chcd3-R_coh_chcd3)
da_coh_chcd3	Total time scale factor, coh	m	r * Dts_coh_chcd3

9.2.3. Subdomain 4-5

Name	**Description**	**Unit**	**Expression**
grad_cl_r_chcd	Concentration gradient, cl, r	mol/m^4	

	component		
dflux_cl_r_chcd	Diffusive flux, cl, r component	mol/(m^2*s)	
cflux_cl_r_chcd	Convective flux, cl, r component	mol/(m^2*s)	
tflux_cl_r_chcd	Total flux, cl, r component	mol/(m^2*s)	
grad_cl_z_chcd	Concentration gradient, cl, z component	mol/m^4	
dflux_cl_z_chcd	Diffusive flux, cl, z component	mol/(m^2*s)	
cflux_cl_z_chcd	Convective flux, cl, z component	mol/(m^2*s)	
tflux_cl_z_chcd	Total flux, cl, z component	mol/(m^2*s)	
beta_cl_r_chcd	Convective field, cl, r component	m^2/s	
beta_cl_z_chcd	Convective field, cl, z component	m^2/s	
grad_cl_chcd	Concentration gradient, cl	mol/m^4	
dflux_cl_chcd	Diffusive flux, cl	mol/(m^2*s)	
cflux_cl_chcd	Convective flux, cl	mol/(m^2*s)	
tflux_cl_chcd	Total flux, cl	mol/(m^2*s)	

cellPe_cl_chcd	Cell Peclet number, cl	1	
Dm_cl_chcd	Mean diffusion coefficient, cl	m^3/s	
res_cl_chcd	Equation residual for cl	mol/(m^2*s)	
res_sc_cl_chcd	Shock capturing residual for cl	mol/(m^2*s)	
da_cl_chcd	Total time scale factor, cl	m	
grad_cg_r_chcd2	Concentration gradient, cg, r component	mol/m^4	cgr
dflux_cg_r_chcd2	Diffusive flux, cg, r component	mol/(m^2*s)	-Drr_cg_chcd2 * cgr-Drz_cg_chcd2 * cgz
cflux_cg_r_chcd2	Convective flux, cg, r component	mol/(m^2*s)	cg * u_cg_chcd2
tflux_cg_r_chcd2	Total flux, cg, r component	mol/(m^2*s)	dflux_cg_r_chcd2+cflux_cg_r_chcd2
grad_cg_z_chcd2	Concentration gradient, cg, z component	mol/m^4	cgz
dflux_cg_z_chcd2	Diffusive flux, cg, z component	mol/(m^2*s)	-Dzr_cg_chcd2 * cgr-Dzz_cg_chcd2 * cgz
cflux_cg_z_chcd2	Convective flux, cg, z	mol/(m^2*s)	cg * v_cg_chcd2

	component		
tflux_cg_z_chcd2	Total flux, cg, z component	mol/(m^2*s)	dflux_cg_z_chcd2+cflux_cg_z_chcd2
beta_cg_r_chcd2	Convective field, cg, r component	m^2/s	r * u_cg_chcd2
beta_cg_z_chcd2	Convective field, cg, z component	m^2/s	r * v_cg_chcd2
grad_cg_chcd2	Concentration gradient, cg	mol/m^4	sqrt(grad_cg_r_chcd2^2+grad_cg_z_chcd2^2)
dflux_cg_chcd2	Diffusive flux, cg	mol/(m^2*s)	sqrt(dflux_cg_r_chcd2^2+dflux_cg_z_chcd2^2)
cflux_cg_chcd2	Convective flux, cg	mol/(m^2*s)	sqrt(cflux_cg_r_chcd2^2+cflux_cg_z_chcd2^2)
tflux_cg_chcd2	Total flux, cg	mol/(m^2*s)	sqrt(tflux_cg_r_chcd2^2+tflux_cg_z_chcd2^2)
cellPe_cg_chcd2	Cell Peclet number, cg	1	h * sqrt(beta_cg_r_chcd2^2+beta_cg_z_chcd2^2)/Dm_cg_chcd2
Dm_cg_chcd2	Mean diffusion coefficient, cg	m^3/s	r * (Drr_cg_chcd2 * u_cg_chcd2^2+Drz_cg_chcd2 * u_cg_chcd2 * v_cg_chcd2+Dzr_cg_chcd2 * v_cg_chcd2 * u_cg_chcd2+Dzz_cg_chcd2 * v_cg_chcd2^2)/(u_cg_chcd2^2+v_cg_chcd2^2+eps)
res_cg_chcd2	Equation residual for cg	mol/(m^2*s)	r * (-Drr_cg_chcd2 * cgrr-Drz_cg_chcd2 * cgrz+cgr * u_cg_chcd2-Dzr_cg_chcd2 * cgzr-Dzz_cg_chcd2 * cgzz+cgz * v_cg_chcd2-R_cg_chcd2)
res_sc_cg_chcd2	Shock capturing residual for cg	mol/(m^2*s)	r * (cgr * u_cg_chcd2+cgz * v_cg_chcd2-R_cg_chcd2)
da_cg_chcd2	Total time scale factor, cg	m	r * Dts_cg_chcd2

grad_cco3_r_chcd3	Concentration gradient, cco3, r component	mol/m^4	
dflux_cco3_r_chcd3	Diffusive flux, cco3, r component	mol/(m^2*s)	
cflux_cco3_r_chcd3	Convective flux, cco3, r component	mol/(m^2*s)	
tflux_cco3_r_chcd3	Total flux, cco3, r component	mol/(m^2*s)	
grad_cco3_z_chcd3	Concentration gradient, cco3, z component	mol/m^4	
dflux_cco3_z_chcd3	Diffusive flux, cco3, z component	mol/(m^2*s)	
cflux_cco3_z_chcd3	Convective flux, cco3, z component	mol/(m^2*s)	
tflux_cco3_z_chcd3	Total flux, cco3, z component	mol/(m^2*s)	
beta_cco3_r_chcd3	Convective field, cco3, r component	m^2/s	
beta_cco3_z_chcd3	Convective field, cco3, z component	m^2/s	
grad_cco3_chcd3	Concentration gradient,	mol/m^4	

	cco3		
dflux_cco3_chcd3	Diffusive flux, cco3	mol/(m^2*s)	
cflux_cco3_chcd3	Convective flux, cco3	mol/(m^2*s)	
tflux_cco3_chcd3	Total flux, cco3	mol/(m^2*s)	
cellPe_cco3_chcd3	Cell Peclet number, cco3	1	
Dm_cco3_chcd3	Mean diffusion coefficient, cco3	m^3/s	
res_cco3_chcd3	Equation residual for cco3	mol/(m^2*s)	
res_sc_cco3_chcd3	Shock capturing residual for cco3	mol/(m^2*s)	
da_cco3_chcd3	Total time scale factor, cco3	m	
grad_cna_r_chcd3	Concentration gradient, cna, r component	mol/m^4	
dflux_cna_r_chcd3	Diffusive flux, cna, r component	mol/(m^2*s)	
cflux_cna_r_chcd3	Convective flux, cna, r component	mol/(m^2*s)	
tflux_cna_r_chcd3	Total flux, cna, r component	mol/(m^2*s)	
grad_cna_z_chc	Concentrat	mol/m^4	

d3	ion gradient, cna, z component		
dflux_cna_z_chcd3	Diffusive flux, cna, z component	mol/(m^2*s)	
cflux_cna_z_chcd3	Convective flux, cna, z component	mol/(m^2*s)	
tflux_cna_z_chcd3	Total flux, cna, z component	mol/(m^2*s)	
beta_cna_r_chcd3	Convective field, cna, r component	m^2/s	
beta_cna_z_chcd3	Convective field, cna, z component	m^2/s	
grad_cna_chcd3	Concentration gradient, cna	mol/m^4	
dflux_cna_chcd3	Diffusive flux, cna	mol/(m^2*s)	
cflux_cna_chcd3	Convective flux, cna	mol/(m^2*s)	
tflux_cna_chcd3	Total flux, cna	mol/(m^2*s)	
cellPe_cna_chcd3	Cell Peclet number, cna	1	
Dm_cna_chcd3	Mean diffusion coefficient, cna	m^3/s	
res_cna_chcd3	Equation residual for cna	mol/(m^2*s)	

res_sc_cna_chcd3	Shock capturing residual for cna	mol/(m^2*s)	
da_cna_chcd3	Total time scale factor, cna	m	
grad_coh_r_chcd3	Concentration gradient, coh, r component	mol/m^4	
dflux_coh_r_chcd3	Diffusive flux, coh, r component	mol/(m^2*s)	
cflux_coh_r_chcd3	Convective flux, coh, r component	mol/(m^2*s)	
tflux_coh_r_chcd3	Total flux, coh, r component	mol/(m^2*s)	
grad_coh_z_chcd3	Concentration gradient, coh, z component	mol/m^4	
dflux_coh_z_chcd3	Diffusive flux, coh, z component	mol/(m^2*s)	
cflux_coh_z_chcd3	Convective flux, coh, z component	mol/(m^2*s)	
tflux_coh_z_chcd3	Total flux, coh, z component	mol/(m^2*s)	
beta_coh_r_chcd3	Convective field, coh, r component	m^2/s	
beta_coh_z_chc	Convectiv	m^2/s	

d3	e field, coh, z component		
grad_coh_chcd3	Concentration gradient, coh	mol/m^4	
dflux_coh_chcd3	Diffusive flux, coh	mol/(m^2*s)	
cflux_coh_chcd3	Convective flux, coh	mol/(m^2*s)	
tflux_coh_chcd3	Total flux, coh	mol/(m^2*s)	
cellPe_coh_chcd3	Cell Peclet number, coh	1	
Dm_coh_chcd3	Mean diffusion coefficient, coh	m^3/s	
res_coh_chcd3	Equation residual for coh	mol/(m^2*s)	
res_sc_coh_chcd3	Shock capturing residual for coh	mol/(m^2*s)	
da_coh_chcd3	Total time scale factor, coh	m	