Chemical Vapor Deposition of MoS$_2$ Rector Design

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Abstract:

Monolayer Molybdenum disulfide (MoS$_2$) is a two-dimensional crystal structure with a direct bandgap which is becoming more popular in the nano-electronics industry due to the semi conductive properties it displays.[1] For this project, we sized and designed a chemical vapor deposition (CVD) system in which a silicon dioxide (SiO$_2$) substrate will be coated by a thin film of MoS$_2$.
Our final design parameters are arrived upon by carrying out sensitivity analysis on several parameters and utilizing kinetic data obtained from literature for the reactions undergoing in the CVD. The semi-batch reactor is designed to be 10dm^3 in volume and the reaction will be carried out at a 175 ^{0}C temperature over the MoO$_3$ boat. Argon, an inert gas, will be flown into the reactor at a rate of 2dm^3/min. With these specifications, the reactor is able to achieve a 91% conversion of the reactants to MoS$_2$ and therefore forming a 7.281 µmoles/dm^3 film layer on the substrate in 15 minutes.

I. INTRODUCTION

Chemical vapor deposition is a promising chemical process which involves a gaseous phase reaction to produce a solid crystal which is deposited on substrate. The deposited crystal improves properties of the substrate such as electrical properties. It has been used in the microelectronic industry to make semiconductor chips. One material of importance in this industry is molybdenum disulfide which is used to improve the semiconducting property of silicon dioxide.

Our objective is to design a chemical vapor deposition reactor for the deposition of molybdenum disulfide on silicon dioxide substrate.

II. NOMENCLATURE

MoO$_3$	Molybdenum Trioxide
MoS$_2$	Molybdenum Disulfide
S	Sulfur
SO$_2$	Sulfur Dioxide
Ar	Argon
MoO$_2$	Molybdenum Dioxide
T	Temperature
P	Pressure
C$_A$	Concentration of Molybdenum trioxide
C$_B$	Concentration of sulfur
C$_C$	Concentration of Molybdenum disulfide
C$_D$	Concentration of sulfur dioxide
-r$_i$	Rate of disappearance of specie i
r$_j$	Rate of appearance of specie j
F$_i$	Flow rate of specie i
N$_i$	Moles of specie i
v_0	Volumetric flow rate
V	volume
H$_i$	Enthalpy of specie i
Cp$_i$	Heat capacity of specie i
Hrxn$_i$	Heat of reaction i
Q	Heat flow
ξ	Extent of reaction
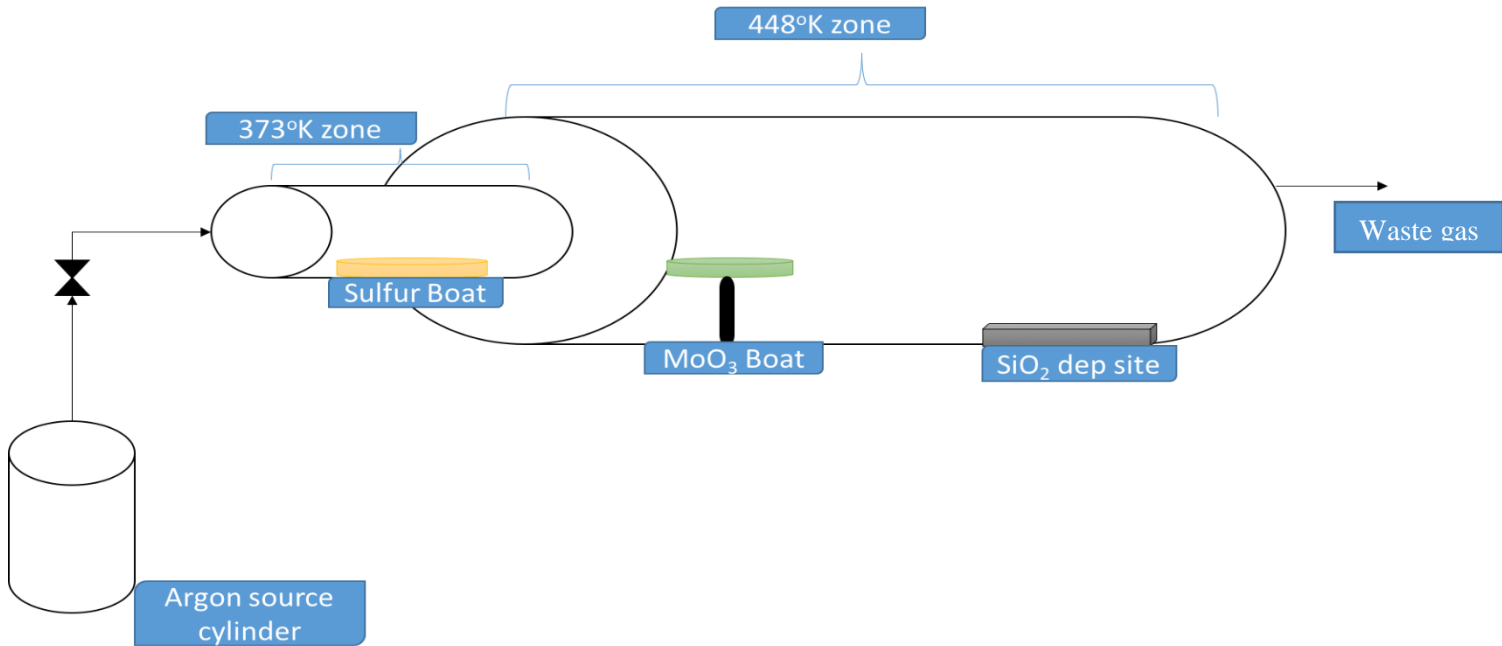
Figure 1: Reactor Schematic

Reaction:

$$2MoO_3 \text{ (s)} + 7S \text{ (g)} \rightarrow 2MoS_2 \text{ (s)} + 3SO_2 \text{ (g)}$$
$$2A \quad + \quad 7B \quad \rightarrow \quad 2C \quad + \quad 3D$$
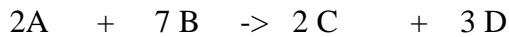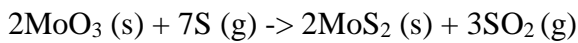
A is the limiting reactant, so we redefine in terms of A

$$A \quad + \quad \frac{7}{2}B \quad \rightarrow \quad C \quad + \quad \frac{3}{2}D$$
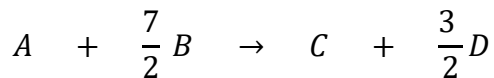
Assumptions:

- Assume no accumulation of Argon/SO_2 gas
- Assume $C_C = C_D = 0$ @t=0
- Assume constant volume
- Assume irreversible kinetics

General Mole balance

In-Out + Generation=Accumulation

Species A

$$0 - 0 + r_A * v = \frac{dN_A}{dt}$$

$$\frac{dN_A}{dt} = r_A * v$$

Species B

$$0 - F_B + r_B *v = \frac{dN_B}{dt}$$

$$\frac{dN_B}{dt} = r_B * v - F_B$$

Species C

$$0 - 0 + r_C * v = \frac{dN_C}{dt}$$

$$\frac{dN_C}{dt} = r_c * v$$

Species D

$$0 - F_D + r_D * v = 0$$

$$F_D = r_D * v$$

Inert

$$F_{i,0} = F_i$$

Rate Law:

$$-r_A = K * C_A^\alpha * C_B^\beta$$

Correlation between rates (via stoichiometry)

$$\frac{-r_A}{2} = \frac{-r_B}{7} = \frac{r_C}{2} = \frac{r_D}{3}$$

So that: $\qquad -r_A = r_C$

$$-r_B = \frac{7}{3} r_D = -\frac{7}{2} * r_A$$

$$C_i = \frac{N_i}{V} \rightarrow\rightarrow\rightarrow N_i = C_i * V$$

$$N_A = N_{A,0} * (1 - x)$$

Where $\qquad$ *X = conversion*

Solve for x:

$$x = \frac{N_{A,0} - N_A}{N_{A,0}}$$

Species A Balance (B-1)

$$r_A * V = \frac{dN_A}{dt} = \frac{d(C_A * V)}{dt}$$

$$\frac{dC_A}{dt} = r_A$$

Species B Balance (B-2)

$$r_B * V - F_B = \frac{dN_B}{dt} = \frac{d(C_B * V)}{dt}$$

Where: $\qquad r_B = \frac{7}{2} * r_A$

$$\frac{dC_B}{dt} = \frac{-v}{V} * C_B + \frac{7}{2} * r_A$$

Species C Balance (B-3)

$$r_C * V = \frac{dN_C}{dt} = \frac{d(C_C * V)}{dt}$$

Where: $\qquad r_C = -r_A$

$$\frac{dC_C}{dt} = -r_A$$

Species D Balance (B-4)

$$v * C_D = r_D * V$$

Where: $\qquad r_D = -\frac{3}{2} * r_A$

$$\frac{v}{V} * C_D = -\frac{3}{2} * r_A$$

Therefore:

B-1

$$\frac{dC_A}{dt} = r_A$$

B-2

$$\frac{dC_B}{dt} = \frac{-v}{V} * C_B + \frac{7}{2} * r_A$$

B-3

$$\frac{dC_C}{dt} = -r_A$$

B-4

$$\frac{v}{V} * C_D = -\frac{3}{2} * r_A$$
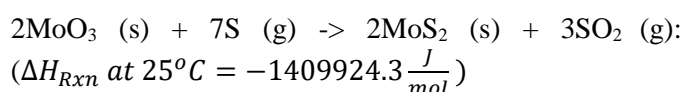
Inert

$$F_{i,0} = F_i$$

General Energy Balance

$$\dot{Q} - \dot{W} + \sum_{in} n_i H_i - \sum_{out} n_i H_i - \sum \xi \Delta H_{rxn} = \frac{dE}{dt}$$

We can now simplify the general energy balance for the reactor with the steady state assumption as the bulk energy is used to heat the inert Argon gas which is at a steady flow and no work is being done on or by the reactor:

$$\dot{Q} + \sum_{in} n_i H_i - \sum_{out} n_i H_i - \xi \Delta H_{rxn} = 0$$

Reaction:

$2MoO_3$ (s) + 7S (g) -> $2MoS_2$ (s) + $3SO_2$ (g):
(ΔH_{Rxn} at $25^oC = -1409924.3 \frac{J}{mol}$)

Heat Capacity[2] ($\frac{J}{mol*K}$)

$Ar_{(g)}$: 20.8

$MoO_{3\,(s)}$: 63.178 + 0.0506T

$S_{(s)}$: 15.188 + 0.0268T

$S_{(g)}$: 35.9 + 0.0013T

$MoS_{2(s)}$: 82.425 + 0.0132T

SO_2 (g): 32.217 + 0.0222T + 3.473E-06T^2

Heat of Fusion[3] & Heat of Vaporization[2] ($\frac{J}{mol}$)

Sulfur:

Heat of Fusion $= 1730 \frac{J}{mol}$

Heat of Vaporization $= 9204.8 \frac{J}{mol}$

Assumptions:

Isothermal Reactor (175ºC)
Isobaric (0.5 torr)
$Tref = 25^oC$

Calculate the enthalpies for each product & reactant:
(sample calculations)

$$H_{Ar} = \int_{298K}^{448K} 20.8 dT$$
$$= 20.8 \frac{J}{mol*K} * (448K - 298K)$$
$$= 3120 \frac{J}{mol}$$

$$H_{MoO_3} = \int_{298K}^{448K} (63.178 + 0.0506T)dT$$
$$= 12309.3 \frac{J}{mol}$$

$$H_S = \int_{298K}^{388.36K} (15.188 + 0.0268T)dT + 1730 \frac{J}{mol}$$
$$+ \int_{388.36K}^{448K} (35.9 + 0.0013T)dT$$
$$+ 9204.8 \frac{J}{mol} = 15310.55 \frac{J}{mol}$$

$$H_{MoS_2} = \int_{298K}^{448K} (82.425 + 0.0132T)dT$$
$$= 13101.12 \frac{J}{mol}$$

$$H_{SO_2} = \int_{298K}^{448K} (32.217 + 0.0222T + 3.473$$
$$* 10^6 T^2)dT = 6146.67 \frac{J}{mol}$$

The ΔHrxn at 175ºC was calculated to be approximately: -1416269.94 J/mol

Moles of components at the end of the 15 minute reaction cycle:

Component	Moles
Ar(g)	1.34
$MoO_{3\,(s)}$	7.19E-06
$S_{(g)}$	7.15E-05
$MoS_{2\,(s)}$	7.28E-05
$SO_{2\,(g)}$	1.09E-04

Calculate the heat flow $Tref = 25^oC$:

The heat flow is calculated using the energy balance listed below along with the enthalpy's listed above, their respective molar flow rates from our mass

balances, the extent of reaction and the enthalpy of reaction listed above:

$$\dot{Q} = \sum_{out} n_i H_i - \sum_{in} n_i H_i + \xi \Delta H_{rxn}$$

$\dot{Q} = 4182.8 \, J - 0 \, J - 103.12 \, J = 4079.68 \, Joules$

Therefore, the heat duty for the 15 minute reaction cycle is $4079.68 \, Joules$.

IV. RESULTS AND DISCUSSION

Reactions, reaction properties and justification of approach for side reaction:

The primary and desired reaction that is taking place in the reactor is the formation of solid MoS_2 and gaseous SO_2 from the reaction between gaseous sulfur and solid MoO_3. This reaction is exothermic with the heat of reaction being $1,409.92 \frac{kJ}{mol}$. This reaction occurs when MoO_3 is partially reduced to an intermediate, in an ideal case the intermediate is MoO_2.[3] Sulfurization of the intermediate then occurs which transforms the ideal intermediate MoO_2 to MoS_2.[3] The intermediate step in this reaction is very fast and is not observed. An assumption is made that the desired reaction will be the only reaction that is occurring in the reactor. The justification of this assumption is discussed below with the required conditions for the possible side reactions.

The assumption that only the desired reaction will occur is justified by the set reactor temperature, pressure, and component concentrations. These reactor parameters inhibit the ability of the possible side reactions from occurring and are discussed below. A possible side reaction could occur to produce the same solid MoS_2 and gaseous SO_2 products from the reaction between solid sulfur and MoO_3. This reaction is endothermic with the

heat of reaction being $148.2 \frac{kJ}{mol}$. This reaction is undesired as it would require a greater input of energy into the reactor. This reaction is assumed to not occur as the reactor is at a constant temperature of 175°C and 0.5 torr and sulfur is a gas at this temperature and pressure. Therefore, no solid sulfur should be present for this reaction to occur. There is another possible side reaction if oxygen is present in the reactor, this side reaction produces solid MoO_3 and gaseous SO_2 from the reaction between solid MoS_2 and gaseous oxygen. This is an exothermic reaction with the heat of reaction being $2,225.89 \frac{kJ}{mol}$. Therefore, if oxygen is present in the reactor then the desired product (MoS_2) will be converted back to a reactant of the desired reaction. To prevent this undesired reaction, the desired reaction is carried out in an oxygen free reactor.

Discussion of Literature Kinetics and determination of the rate law r_A:

As a wrong, but unavoidable assumption, rate law was mentioned earlier, and will be elaborated upon here. There is a scarcity of data comparing film thickness and accumulation with time, with only two sources coming close. Instead, most papers are concerned with the properties of the film, such as binding energy[4], electric properties[5], or even the volume and size of the individual molecules.[6] Intensity vs. Raman shift is very often measured as well, even occasionally as a function of time[7]. Intensity is directly proportional to concentration, but a mathematical relationship between the two was not found. One of the two promising sources is behind a paywall, and was unable to be accessed. Instead, the other source[8] was used, which does not include volume or concentration. This means that even though it is possible

to calculate the rate law, it is impossible to calculate the rate constant if we assume a first order reaction. Because of this, once the rate law is calculated, it is necessary to assume a zero order reaction to complete the models. In the future, there should be more kinetic data available, and the study can be reopened. Data for the film thickness with respect to time is not tabulated, so it had to be interpreted from graphics.[8] The first thickness and number of cycles in Table II are recorded data, the rest are simple unit conversions.

Table II: Thickness with respect to time

Thickness (nm)	# of cycles	Total time (min)	nm/min	cm/min
5	100	50	0.1	0.00000001
10	200	100	0.1	0.00000001
14	300	150	0.093333	9.3333E-09
23	500	250	0.092	9.2E-09
27	600	300	0.09	9E-09

The specifications given in the paper assume a basic cycle @ 175 °C and a pressure of 0.5 Torr.

Because the paper does not directly model our experiments, a few more assumptions are made. First of all, the data is derived using pulsing cycles as listed[8]:

20 seconds of pumping MoO_3 gas

10 seconds of purging with argon gas

30 seconds of pumping sulfur gas

10 seconds of purging with argon gas

MoO_3 is the reactant closer to the reaction site in our reactor. Argon and sulfur gas are flowed over the MoO_3 and the reaction site. Because MoO_3 is the limiting reactant, and because it is closer to the reaction site, we assume that we have a constant flow of sulfur with regards to the data experiment. This means that we take a cycle as the 30 seconds of pumping sulfur. These calculations were used in Table II.

Next, we need to calculate the volume deposition. Per the data source[8], all wafers used are uniform circles with 4-inch diameter.

Thus, the area is:

$$A = \pi * r^2 = \pi * 2^2 = 12.56636 \; inches$$

Converting to square centimeters yields:

81.073128176 cm².

Finally, the volume rate of deposition of MoS_2 for each case shown in Table III:

Table III : Deposition for all trials

cm/min	Volume/min
0.00000001	8.107E-07
0.00000001	8.107E-07
9.33333E-09	7.56653E-07
9.2E-09	7.45844E-07
0.000000009	7.2963E-07

This gives an average MoS_2 volume increase of 7.70705E-07 cm³/min.

As a solid, an assumption is made that the density does not vary much with temperature.

Hence, the density of MoS_2 is 5.06 g/cm⁸. We can then find the rate of gram deposition:

$$\frac{5.06 \; g}{cm^3} * \frac{7.70705 * 10^{-7} cm^3}{min} = 3.9 * 10^{-6} \frac{g}{min}$$

This is then converted into a molar rate using the molar mass of MoO_3:

$$\frac{3.9 * 10^{-6} \; g}{min} * \frac{mol}{160.7 \; g} = 2.43 * 10^{-8} \frac{mol}{min}$$

This is the molar growth rate of MoS_2.

This is where we run into the first major problem. Unfortunately, no volume, concentration, mole value, or conversion is listed for the initial quantity of MoO_3. Thus,

stoichiometry is used to find the rate of decay of MoO_3. This is the limiting reactant, and the rate law we are trying to calculate.

$$-r_A = r_C$$

Hence, rate of decay of MoO_3 is

$$-2.43 * 10^{-8} \frac{mol}{min}$$

Knowing that the MoO_3 is carried in 50 standard cubic centimeters per minute of argon gas,[8] and assuming it evenly disperses through the gas, it should adopt the entire volume of the argon gas. This is not a very good assumption, but the best available, as no other estimate for the powder volume (or the quantity of powder that reacts) is given. Hence, the concentration rate of decay of MoO_3:

$$-2.43 * 10^{-8} \frac{mol}{min} * \frac{1}{50 \ cm^3}$$

$$= 4.853 * 10^{-10} \frac{mol}{cm^3 * min}$$

Finally, this must be converted to standard units:

$$4.853 * 10^{-10} \frac{mol}{cm^3 * min} * \frac{10^3 \ cm^3}{1 \ dm^3} * \frac{1 \ min}{60 \ seconds}$$

$$= 8.090 * 10^{-9}$$

This gives a final rate law of:

$$r_{MoO_3} = 8.090 * 10^{-9} \frac{mol}{dm^3 * s}$$

This is the rate of reaction in terms of the limiting reactant, MoO_3

$$r_{MoS_2} = -8.090 * 10^{-9} \frac{mol}{dm^3 * s}$$

$$r_B = -2.8315 * 10^{-8} \frac{mol}{dm^3 * s}$$

$$r_C = 8.090 * 10^{-9} \frac{mol}{dm^3 * s}$$

$$r_D = 1.2135 * 10^{-8} \frac{mol}{dm^3 * s}$$

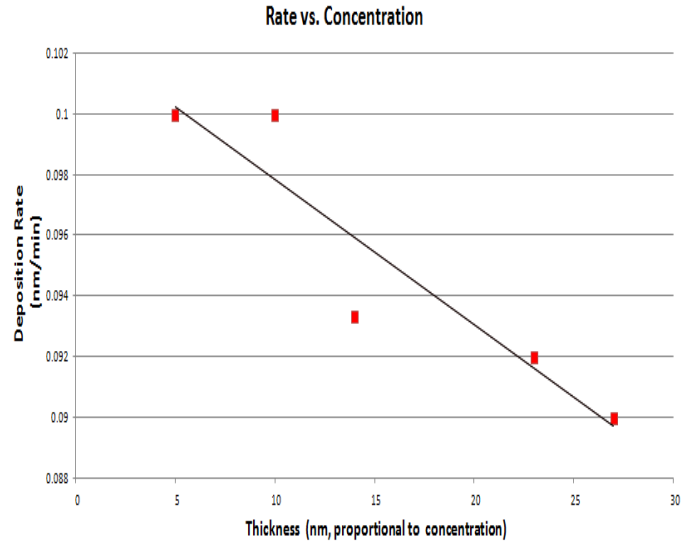Per the paper[8], the rate continues to change linearly as seen in Figure 2.

Figure 2- Rate of deposition (rA) with respect to thickness

However, because we do not know the initial concentration or volume of the reaction area, we must plot and compare the deposition rate with the thickness, as thickness should be proportional to concentration. Each point represents a different reaction duration. What this shows is that there is a linear correlation between rate and concentration, which implies a first order reaction assuming the form of:

$$-r_A = k * C_A$$

Again, because of a lack of data, we must assume a zero order reaction, per power law, in which case:

$$-r_A = k * C_A^0 = k$$

This rate law is used for all calculations, including conversion.

The other kinetic information garnered from literature is that we do not require a catalyst. This was decided as the rate data[8] does not use a catalyst, and catalysts in CVD are mostly used with carbon nanotubes. Some potential but unexplored catalysts are nickel, iron,

and cobalt[9], which could theoretically decrease operating temperature.

Assumptions and Justifications:

Argon is inert

As a noble gas, Argon is considered inert in the reaction. A further assumption is that there is no accumulation of argon due to continuous flow.

Sulfur Dioxide does not accumulate

In the material balance, the concentration of sulfur dioxide remains zero. This is because as it is being generated, it is being removed from the reactor with the argon gas.

Initial product concentration is zero.

Another assumption, made for mass balances, is that at the start of the process, there is no product, MoS_2 or SO_2, at the reaction site. This holds true as long as proper purging is observed. The reaction site is replaced, and residual SO_2 is removed with the carrier gas.

Assuming Constant Volume

Due to a low mole fraction of 0.036 for the limiting reactant, MoO_3, the gas expansion factor should be negligible, and gas volume will not change significantly.

Irreversible Reaction

Because the rate data[8] failed to mention a reversible reaction, we assume that at the given temperature and pressure, the reverse reaction either does not occur, or is already calculated into the rate data.

Furthermore, with no oxygen, there is no chance for the side reaction to occur[10].

Isothermal Reactor

Even though the reactor tube contains a temperature gradient, due to reaction requirements, the reaction site is at constant temperature. A temperature gradient is required for the chemical vapor deposition process[5], and using this source, our temperatures are chosen, with the sulfur boat at 100 °C and the reaction site at 175 °C. Because the reaction site is held at constant temperature, the temperature gradient of the reaction site itself will be negligible.

Pressure does not affect energy balance

The rate data has the pressure in the reactor at almost vacuum value, 0.5 Torr[8]. We assume that because enthalpy is not strongly affected by pressure, that this pressure does not have a significant change from reference enthalpy.

All MoS2 binds to silicon

Because rate data is given in terms of thickness on the wafer, it only measures the amount of MoS_2 that actually binds to the substrate. Unfortunately, because of a lack of information, such as the initial moles of MoO_3, we do not know the ratio of MoS_2 that flows out of the reactor and missing the silicon platform. One source[5] depicts the MoO_3 substrate located directly beneath the silicon platform, performing the deposition "upside down". This theoretically increases MoS_2 retention. However, this assumption is inherently imperfect, so the film thickness in real world scenarios will be decreased.

<u>Zero Order Kinetics</u>

The final and arguably worst assumption is that this reaction uses zero order kinetics. This is born out of necessity other than choice. The rate data[7] found implies a first order reaction, as shown in the rate calculations section of the paper. There is a lack of information around the kinetics of the reaction, notably the failure for the sources to show initial volume, mass, or concentration[7]. Other sources failed to give thickness as a function of time[4,5,6,7]. No sources gave concentration as a function of time, or derived kinetics. Because of this, rate law is calculable, but we cannot calculate the mass balances with respect to a first order reaction. This requires the initial concentration, and thus we can only calculate assuming a zero order reaction. This will be elaborated upon in the section discussing the kinematics and rate law.

Results of Material Balance:

Once rate law is determined, and a zero order reaction is chosen, all reactor information was imported into Matlab, as explained in Appendix A. This base rate can be scaled due to reactor temperature based on the Arrhenius model[11], but we will use a temperature of 448K, like the one used for rate data[7]. Volumetric flow rate of argon, and reactor volume are both specified, with base values of 2 dm^3/min and 10 dm^3, although these are easily adjusted in the code.

With an initial feed of $8 * 10^{-6}$ moles of MoO_3, and baseline values kept for argon flow and reactor volume are tabulated in Table IV.

Table IV – Results for a sample test of reactor

Time (min)	MoO_3 (moles/dm³)	S_2 (moles/dm³)	MoS_2 (moles/dm³)	SO_2 (moles/dm³)	Conversion
0	8.00e-6	2.10e-04	0.0	0.0	0.0
4	6.06e-06	8.97e-05	1.94e-06	3.64e-06	0.24
8	4.12e-06	3.56e-05	3.88e-06	3.64e-06	0.49
12	2.18e-06	1.13e-05	5.82e-06	3.64e-06	0.73
15	7.19e-07	2.38e-06	7.28e-06	3.64e-06	0.91

It is important to note that all of the variables can be easily changed for different conversions. 91% conversion was chosen as a desirable number, although keep in mind that this number is greater than a real life scenario, as mentioned in the assumptions section. Due to the zero order assumption, there is no limit to conversion, and it will continue to increase as long as there is enough limiting reactant. Figures 4 and 5 are also obtained:

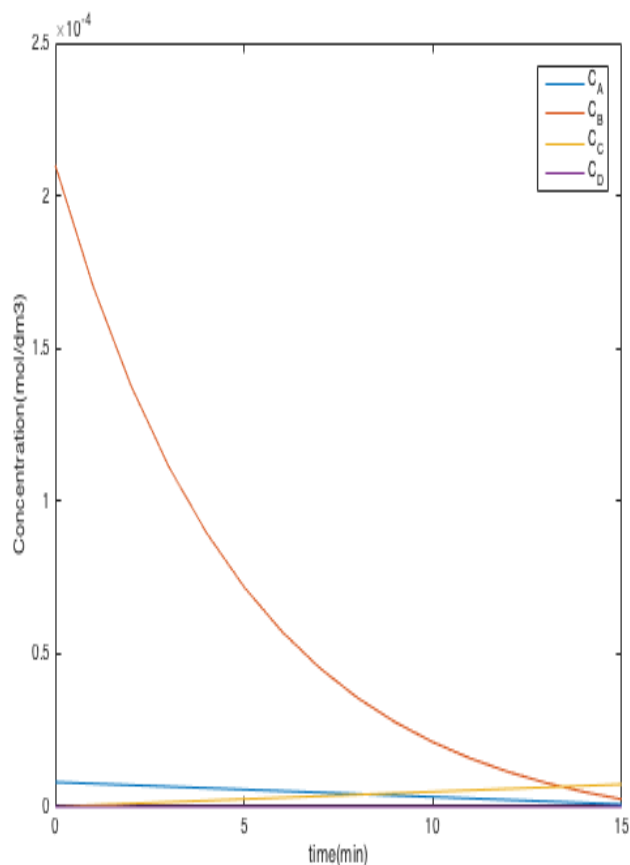**Figure 4** – Concentration of all compounds vs. time.

Figure 5 – Conversion of MoO3 as a function of time.

This is for the specified sample test. Note how the concentration of MoO_3 appears to be linear; this is because of the zero order assumption. It is also important to note how much faster the concentration of sulfur decreases, this is why so much is required, and we run it in excess. The concentration of SO_2 will remain zero, as we are assuming that all that is generated is removed from the reactor with argon.
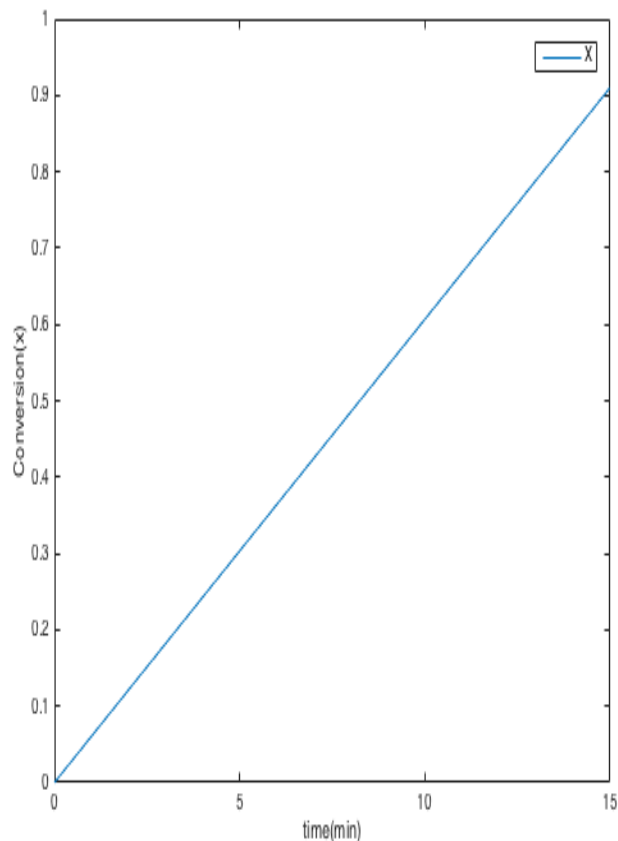
This shows a straight line, as we have to assume a zero order reaction. Because of this, the conversion will always reach 100%, as long as there is enough time. Unfortunately, maximum conversion is very unlikely to be accurate, so about 91% is chosen for the sample test for a more realistic view.

If a first order reaction could be calculated, the concentration of MoO_3 in Figure 4 would appear exponential as opposed to linear, and the conversion would appear to be a logarithmic graph, with a maximum conversion appearing at the asymptote. As mentioned, if the project was to be undertaken again, accurate rate data would drastically increase the accuracy of the report.

Energy balances results and analyses:

The energy balance based on a single desired reaction which is exothermic. The general energy balance was simplified by assuming there is no work put into or removed from the system. The energy balance was also further simplified by assuming a steady state energy balance, this was assumed as the bulk flow of energy is due to the flowing argon gas which is not accumulating in the system. The reactants are charged into the reactor at 25°C then it is brought to 175°C by adding ~4182.8 joules for the 15 minute reaction cycle. The section where the sulfur boat is located is only heat heated up to 100°C while the molybdenum trioxide section is the hottest zone.

Once the temperature stabilizes at 175°C, the carrier gas is made to flow thereby bring the reactants into the hottest section of the reactor where the reaction occurs. Since the reaction is the reaction is exothermic and gives of ~103.12 joules of heat over the course of the reaction cycle, the heat input to system is reduced to ~4079.68 joules. This done to keep the reactor isothermal at 175°C.

Sensitivity Analysis:

Sensitivity analysis was conducted by changing Temperature, volumetric flow of the carrier gas, and reactor volume. The variable of interest was the conversion of the molybdenum trioxide which was in limited amount. We found that conversion is very sensitive to the operating temperature and increases with increasing temperature. We also found that the volume of reactor since assumed independent of time had no effect on the conversion of the limiting reactant(MoO_3). However, increasing the volumetric flow rate of the carrier gas, increases the rate at which sulfur in the gas phase is removed from reactor, thereby making it the limiting reactant, and increasing waste.

Figure 6 below, shows concentration changing with time when the temperature of the system is maintained at 450K. Conversion is very low at this temperature. Figure 7 shows high conversion at 450K which is expected since rate increases with increasing temperature.
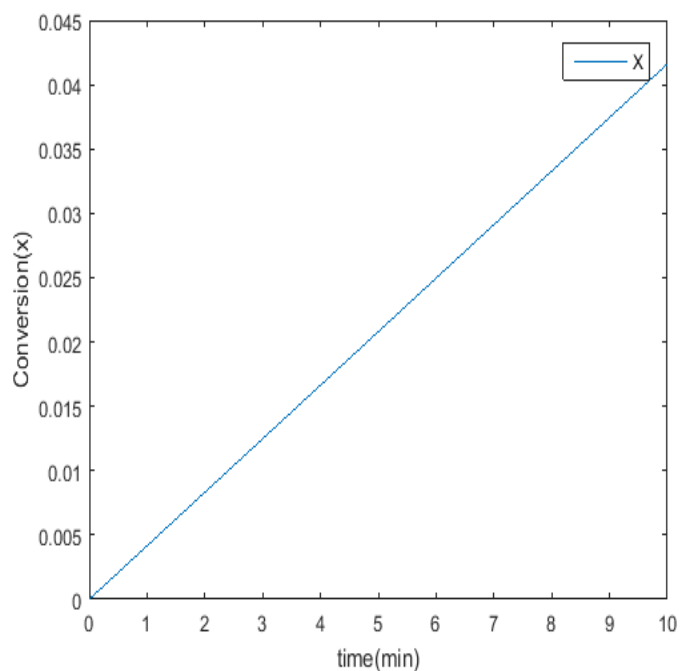

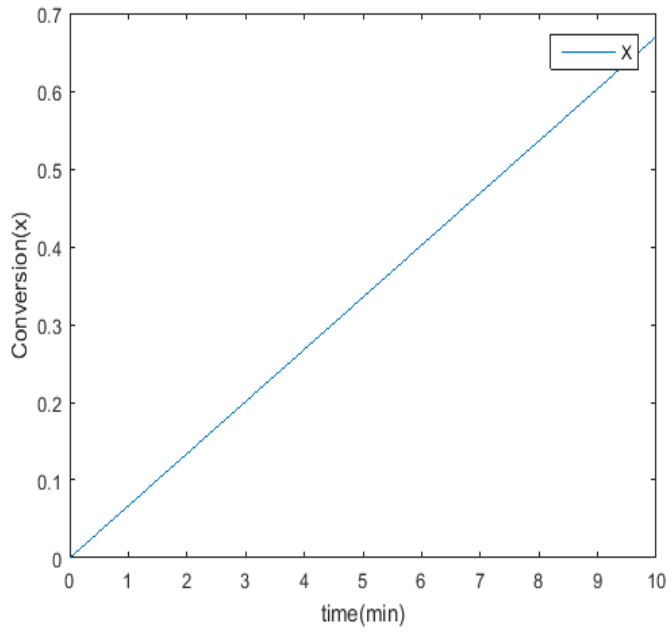**Figure 6**: Conversion versus time at T = 400K

Figure 7: Conversion versus time at T = 450K

Figure 8: Concentration versus time at $T = 450K$ and $v_0 = 1\ dm^3/\min$

Figure 8 and 9 below shows the effect of changing the flow rate of the carrier gas. In figure 8, the flow rate is 1dm³/min and 4dm³/min in figure 9. The concentration of sulfur drops rapidly as the volumetric flow rate of the carrier gas is increased. The concentration of molybdenum disulfide and molybdenum trioxide is not affected because it is assumed that they remained in the solid phase through the course of reaction therefore negligible amount is lost.
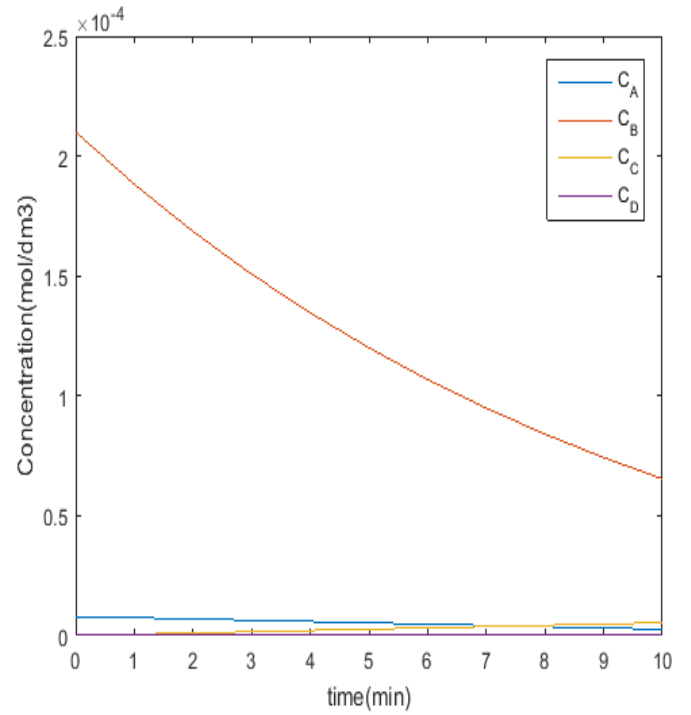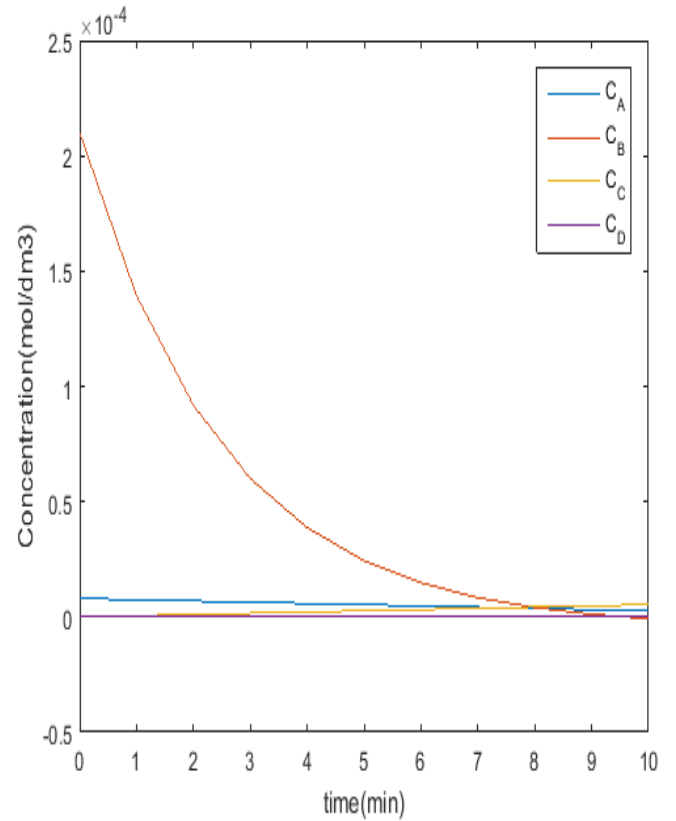

Figure 9: Concentration versus time at $T = 450K$ and $v_0 = 4\ dm^3/\min$

Anticipated scale of design:

The volume of the semi- batch reactor and initial concentrations of the reactants were decision variables which were selected after carrying out some research and material balance calculations with various volumes of the reactor and initial concentrations[6]. We selected the variables which yielded the best results for the final concentration of MoS_2 film in the reaction.

- The length of the tubular reactor where reaction will be taking place is 100 cm with a 11.3 cm diameter.
- The limiting reactant in this process is the MoO_3 with an initial concentration of 8×10^{-6} mol/dm^3
- Excess Sulfur is present in the reactor with an initial concentration of 2.1×10^{-4} mol/dm^3
- With this scale, 7.281 µmoles/dm^3 of MoS_2 film will be formed on the silicon dioxide substrate in 15 minutes.

Safety Considerations:

The precursors (MoO_3 and S) and the by-products in Chemical vapor deposition processes are toxic, pyrophoric, corrosive and also flammable. Therefore, skin and eye contact must be avoided at all times by wearing goggles, gloves and protective clothing. Precaution must also be taken when handling pressurized tank components such as valves, regulators and piping as they can corrode and cause burns to the skin[14]. These pressurized tanks should also be stored in cool, dry, well ventilated and fire resistant areas to avoid explosions of the tanks. Lastly, the exhaust systems of a CVD contain abrasive particulates and corrosive/toxic species. Proper ventilation must be available and careful handling/discharge of the species is required as the particulates and corrosive species are not only harmful to humans but also the environment. Less toxic precursors can be utilized to avoid such problems.[13]

V. CONCLUSIONS

We concluded that based on the zero order kinetics:

- Chemical vapor deposition of MoS_2 can be carried out at 448K and 0.5 torr with high yield of MoS_2.
- Chemical vapor deposition of MoS_2 is an energy intensive process.
- Temperature controls the conversion of MoO_3.
- Volumetric flow of the carrier gas needs to 2dm^3/min or less to ensure that less waste is generated.

VI. RECOMMENDATIONS

We recommend:

- Getting access to more data to reduce the amount of assumption.
- Test if a batch or continuous process would give better results
- Performing experiment to get the rate law/data

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APPENDIX   A

The m-file used to carry sensitivity study is name run_final.m. It prompts for temperature, volumetric flow rate, initial concentration of the limiting reactant(MoO_3), and the time to run the reaction. It calculates the concentration of Sulfur in 750% percent excess of the stoichiometric amount.

It produces two plots after each run, concentration versus time and conversion versus time. When the test is terminated by entering -1 for temperature a plot of rate versus temperature is generated