

Calculation of Zinc Pressure

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1 Introduction and Background

The purpose of this document is to describe the way in which the zinc vapor pressure within our system (the Easy Bake Oven) is understood and calculated. Be aware of units during your calculations and note that many of the values contained in the below equations are experimentally determined. Finally, these calculations are not exact and should not be used in an official capacity without further scrutiny and investigation into significant figures and approximations. If using a configuration that varies greatly from the “typical” experiment, your greatest resource are previous experiments which may more closely resemble your set-up. These experiments may offer different values for percentage of zinc absorbed, α , or the aperture of the crucible, among other variables.

2 Measuring Zinc Pressure

In order to measure the partial pressure of zinc during an experiment you must record

1. the mass of the zinc before the experiment begins

2. the mass of the zinc after the conclusion of the experiment
3. the time during which the zinc was evaporating
4. the pressure of the system during growth
5. the temperature of the system during growth
6. the flow rates of all gases into the system.

Use the first three elements of information to calculate the average evaporation rate, E_{Zn} , of zinc (in grams/minute). Next, we assume that only 70% of the zinc that is evaporated actually passes through the quartz tube. This percentage is an estimate based on visual inspection of zinc that condenses on the quartz tube up- and downstream; thus, it can vary greatly depending on the experimental set up. Converting from grams/minute to sccm gives us a factor of 342.6 (calculated in Appendix). This yields an expression for the flow rate of zinc,

$$F_{Zn} = E_{Zn}(.7)(342.6). \quad (1)$$

We can now use the flow rate of zinc to calculate the zinc partial pressure, P_{Zn} ,

$$P_{Zn} = \frac{F_{Zn}}{F_{tot}} P_{tot}. \quad (2)$$

3 Predicting Zinc Evaporation Rate

The logarithmic relationship between zinc vapor pressure and temperature has been experimentally determined by *Klimova, et. al* to be,

variable	definition	units
F_{Zn}	flow rate of zinc	sccm
F_{tot}	flow rate of H, Zn, NH ₃	sccm
E_{Zn}	evaporation rate of zinc	g/min
P_{Zn}	experimental zinc vapor pressure	atm
P_{Zn}^{eq}	equilibrium vapor pressure of zinc	Torr
T	temperature	K
α	constant	g/(min*atm*mm ²)
A	area of crucible opening with lid on	mm ²

$$\log_{10}(P_{Zn}^{eq}) = \frac{-6224}{T(K)} + 8.096. \quad (3)$$

Note that this relationship is only valid under certain assumptions, mainly that the zinc pressure and the equilibrium pressure inside the crucible be the same and that the zinc be evaporating into a volume with a relatively low zinc pressure. This has been the case for the majority of experiments conducted in Kash Lab, but could cause severe over- or underestimation if the conditions of an experiment render this approximation invalid. T in this case refers to the temperature read out by the zinc thermocouple, not the temperature within the furnace. If a specific T is desired in your experiment, you must adjust the zinc crucible position relative to the furnace. It will be necessary to wait approximately 15 minutes for the temperature to settle and you may have to move the crucible several times in order to find the ideal T . The evaporation rate of zinc is given by

$$E_{Zn} = \alpha A P_{Zn}^{eq}(T), \quad (4)$$

where α is just a proportionality constant that has been experimentally determined to be 0.003559 (uncertainty unknown) by E. Blanton. This value of α may be dependent on any number of factors such as the geometry of the zinc crucible and lid, as well as the configuration of the crucible and sample.

variable	definition	value	units
Q	volumetric flow rate	–	sccm
m	mass of one mol of zinc	65.37	g
n	number of moles of gas	1	–
P	standard pressure	1	atm
R	gas constant	82.1	$\frac{\text{cm}^3 \text{atm}}{\text{molK}}$
T	room temperature	273.15	K
m'	mass flow rate	–	g/min

4 Appendix

To convert from sccm to g/min we begin first with the ideal gas law,

$$V = \frac{nRT}{P} \quad (5)$$

which when coupled with the definition of gas density generates the expression,

$$\rho = \frac{mP}{nRT}. \quad (6)$$

Clearly, the volumetric flow rate is the mass flow rate divided by the density of the gas,

$$Q = \frac{m'}{\rho}, \quad (7)$$

and therefore

$$Q = \frac{nRT}{mP} m' \quad (8)$$

which for zinc becomes

$$Q = 342.6 m'. \quad (9)$$

5 Acknowledgements

Data on the vapor pressure of zinc relating to temperature was obtained by the paper "Investigation of the Saturated Vapor Pressure of Zinc, Selenium, and Zinc Selenide", by A.M. Klimova, V.A. Ananichev, Mohammad Arif, and L.N. Blinov (*Glass Physics and Chemistry*, Vol.31, No.6, pp.760-762). Determination of α as well as general procedure achieved by E.Blanton.