Final Report on
Vacuum Drying of Grapes

Grapes, vacuum drying, moisture content, shrinkage, optimization

Digital Food Physics and Engineering BEE 4630/6630
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1. Executive Summary

The high moisture content of grapes leads to a low shelf life, making drying an ideal method for preservation. The global market size for raisins (the term for dried grapes) was estimated at $2.6 billion in 2022 and is predicted to reach $4 billion by 2030 (Wang et al., 2017). It is critical to optimize the raisin production process. Grape skins have a low diffusivity, posing a huge obstacle for drying (Esmaiili et al., 2022). Grapes are often pretreated prior to drying to increase the skin diffusivity and significantly lower drying times (Adiletta et al., 2016). Moreover, vacuum drying is becoming an increasingly popular method for removing grape moisture (Esmaiili et al., 2022). We used COMSOL to investigate the effect that grape skin diffusivity and temperature has on a grape vacuum drying process. Our results agreed with the current literature on the effects that skin diffusivity has on grape drying, but disagreed when it came to temperature effects. Future simulation refinement and deeper literature review is needed to confirm these results.

2. Introduction

2.1 Pretreatments

Grape skin prevents moisture from leaving the pulp due to its low diffusivity. Grapes are often chemically or physically pretreated prior to the drying process to break down the skin. Chemical pretreatments such as ethyl oleate and potassium carbonate create micro-fissures on the skin surface which leads to nonuniform skin removal, while physical pretreatment involves abrasion of the skin surface and results in uniform removal of the skin from the grape (Vakula et al., 2019). Skin diffusivity on untreated grapes can be as low as $1x10^{-22}$ m^2/s to $1x10^{-18}$ m^2/s but can increase to as high as $1x10^{-12}$ m^2/s to $1x10^{-10}$ m^2/s after pretreatment. On the other hand, pulp diffusivity ranges from $1x10^{-10}$ m^2/s to $1x10^{-9}$ m^2/s (Saravacos et al., 2001).

2.2 Vacuum Drying

Fruit has been commonly dried by convective hot air, but vacuum drying has shown significant advantages since it creates a low moisture and low pressure environment where less heat is needed. It also preserves the initial shape and reduces damage of heat-sensitive compounds (Sokač et al., 2022).

2.3 Project

The purpose of this project was to simulate a grape under isobaric vacuum drying conditions and investigate how pretreatments and temperature affect drying times. We used COMSOL to simulate drying at every order of magnitude for skin diffusivity between $1x10^{-22}$ m^2/s and $1x10^{-10}$

m^2/s at a constant temperature of 70°C. We then compared drying at 35°C, 50°C, and 70°C for a constant skin diffusivity of $1x10^{-10}$ m^2/s.

3. Methods

3.1 Problem Setup

We began with a general, pictorial representation of the process and simplifying assumptions, as shown below in Figure 1.

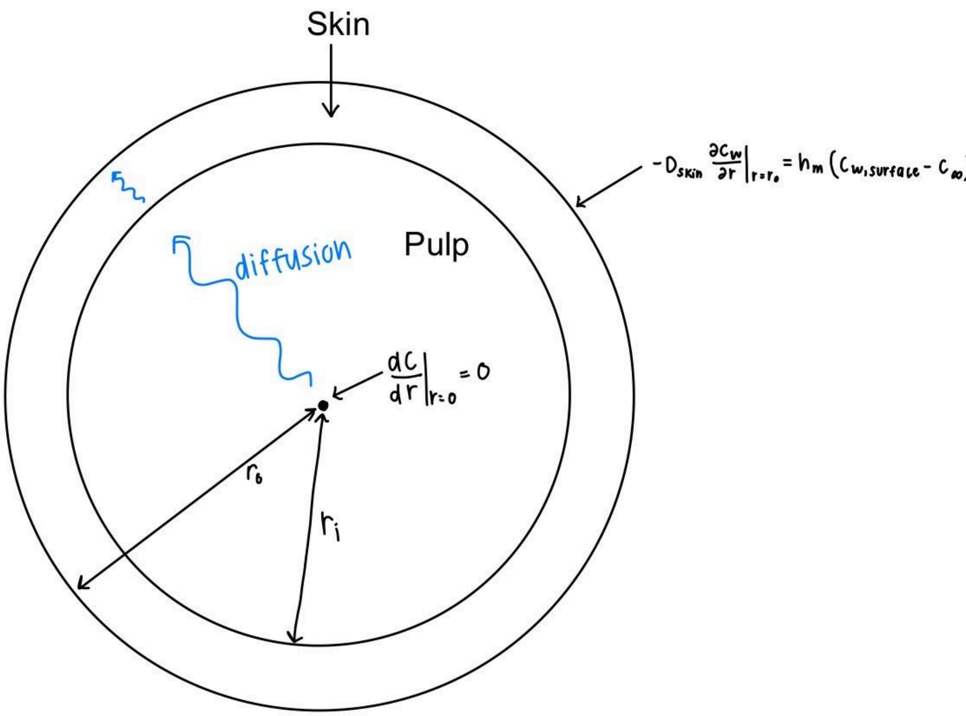

Fig 1*: Schematic of grape drying problem.* We assumed moisture moves outward radially from the grape via diffusion and that the outer skin is subject to convective flux. The pulp radius is denoted as r_i and the skin radius is r_o. The radial flux at the center of the grape is zero, as equal flux occurs in every direction.

We then further defined our flux equations to input into COMSOL, as shown below. Grape pulp diffusivity was calculated using Equation 2 from Saravacos et al., 2001. We ran a simulation with skin diffusivity at every order of magnitude between $1x10^{-22}$ m^2/s and $1x10^{-10}$ m^2/s.

$$\frac{\partial c_A}{\partial t} = D_{AB} \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial c_A}{\partial r})$$

Eqn 1: *Governing equation for mass transfer of water through grape.* We assumed radial diffusion to be the only mass transfer process within the grape. Moisture content is denoted as c_a. The pulp and skin will have different diffusivity D_{AB} values.

$$D = \frac{1}{1+X} D_o \exp\left[-\frac{E_o}{R}\left(\frac{1}{T} - \frac{1}{T_r}\right)\right] + \frac{X}{1+X} D_i \exp\left[-\frac{E_i}{R}\left(\frac{1}{T} - \frac{1}{T_r}\right)\right]$$

Equ 2: *Pulp diffusivity.* Taken from Saravacos et al., 2001. X represents the pulp moisture content, T is the vacuum dryer temperature, and all other values are provided from the source.

$$- D_{skin} \frac{\partial c_A}{\partial r}\Big|_{r=r_o} = h_m(c_{A, surface} - c_\infty) = h_m(\frac{P_v a_w}{RT} - c_\infty)$$

Eqn 3: *Convective boundary condition on the outer grape skin.* We assumed convection to be the only mass transfer process at the skin surface. The moisture concentration at the surface can be assumed to be saturated and can be calculated using the ideal gas law multiplied and the water activity. Pressure and temperature were set using standard vacuum dryer conditions, and the concentration at infinity was set to zero. The water activity was determined using interpolation from Hermassi et al., 2017

The water activity in Equation 3 was determined via interpolation using isothermal water activity data from Hermassi et al., 2017, as shown in Figure 2 below. Although we changed temperatures at different points in the simulation, we always used interpolation for the data at 70°C for the sake of simplicity. The grape internal temperature was also assumed to be the same as that of the external environment. Our interpolation is shown in Figure 3 below. Conversely to the researchers, we found water activity as a function of moisture content. COMSOL tracks the moisture content at each point in the grape throughout the simulation.

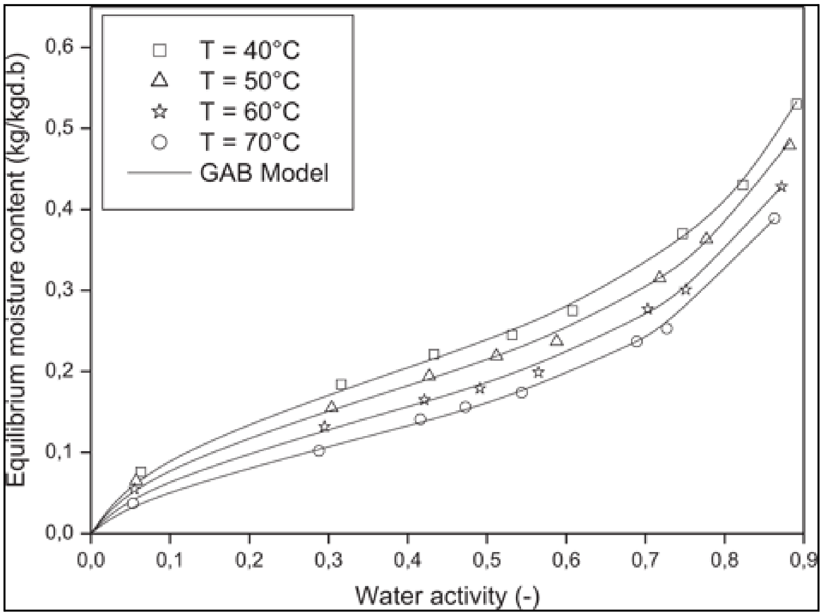

Fig 2: *Moisture content as a function of isothermal water activity for grapes*. This graph shows how Hermassi et al, 2017 were able to accurately model moisture content using water activity. We did not use their model, but we used this data to interpolate the water activity from moisture content.

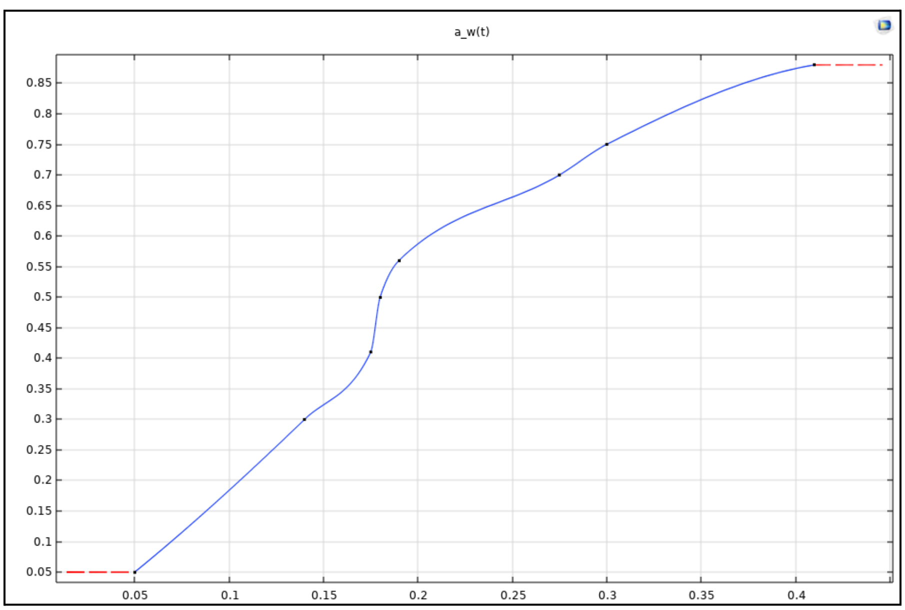

Fig 3: *Interpolated water activity as a function of moisture content.* Water activity is on the y-axis and moisture activity is on the x-axis. Constant extrapolation was used at the highest and lowest moisture content values to prevent water activity from going above 1 and below 0.

As a grape dries to a raisin, its volume shrinks as a result of the moisture loss. We assumed that the grape would shrink uniformly and that the volume decrease would be exactly equal to the amount of moisture lost. To simplify the simulation we also assumed that the moisture in the grape pores was entirely in the liquid phase and no vapor was present.

3.2 COMSOL Setup

The simulation was implemented using COMSOL's Transport of Diluted Species (tds) physics in the 2D-Axisymmetric model wizard as a time-dependent study. The geometry was built using COMSOL's difference feature between two half circles. A 10mm half circle was cut by an overlaid 9.998mm half circle to create one half circle with two different regions. The inner region represented the grape pulp, from 0.0mm to 9.998mm, while the outer 2.0μm represented the grape skin, as shown in Figures 4 and 5 below. A half circle was used instead of a full circle to save computational running time. By default, the 2D-Axisymmetric model wizard applies a zero flux boundary condition on the axis of symmetry, satisfying our inner boundary condition. We assumed the grape to weigh 5g with a moisture content of 81.3% using data from Deer et al., 1989 and Šuklje et al., 2012, resulting in an initial moisture content of 54000.00 mol/m^3.

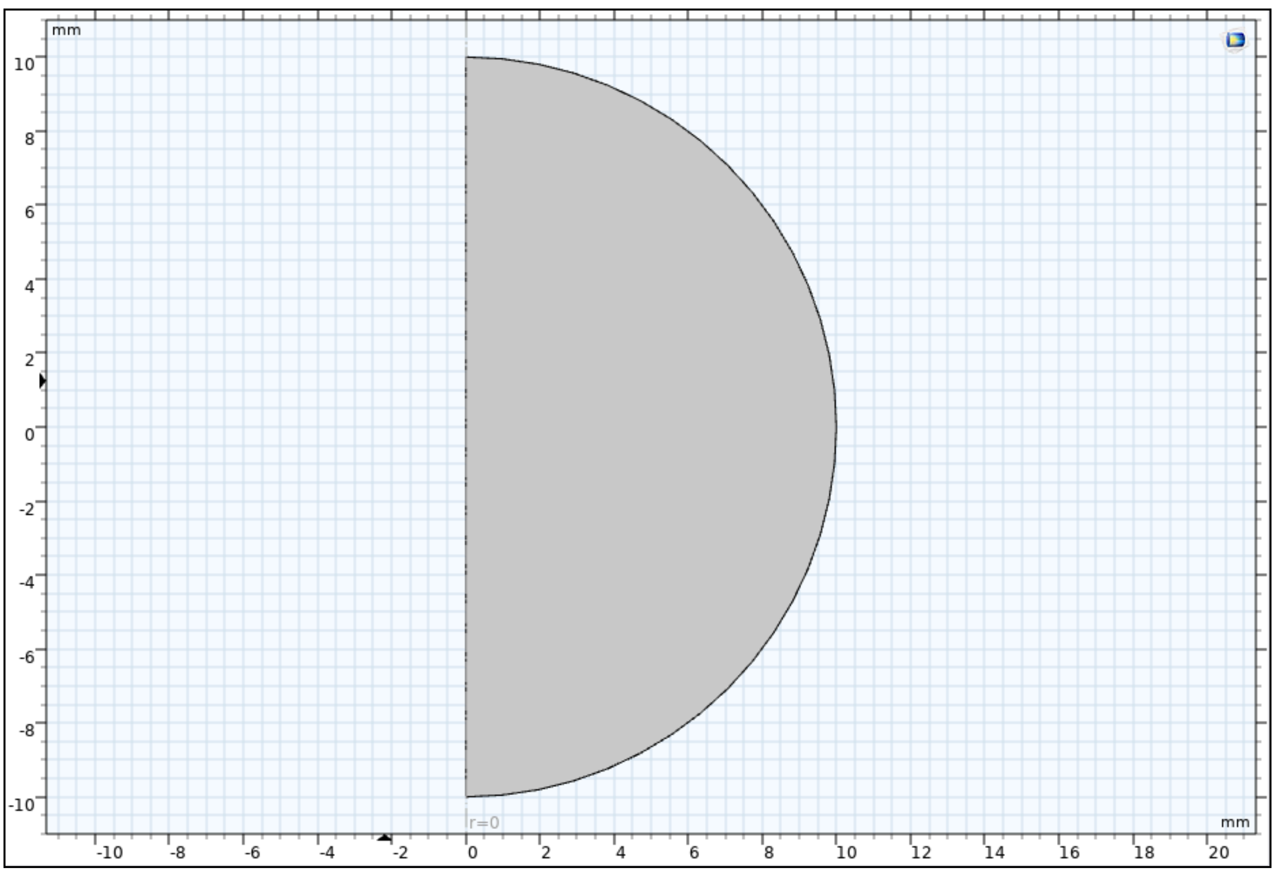

Fig 4*: Complete view of grape pulp and skin.* The total radius was 10 mm.

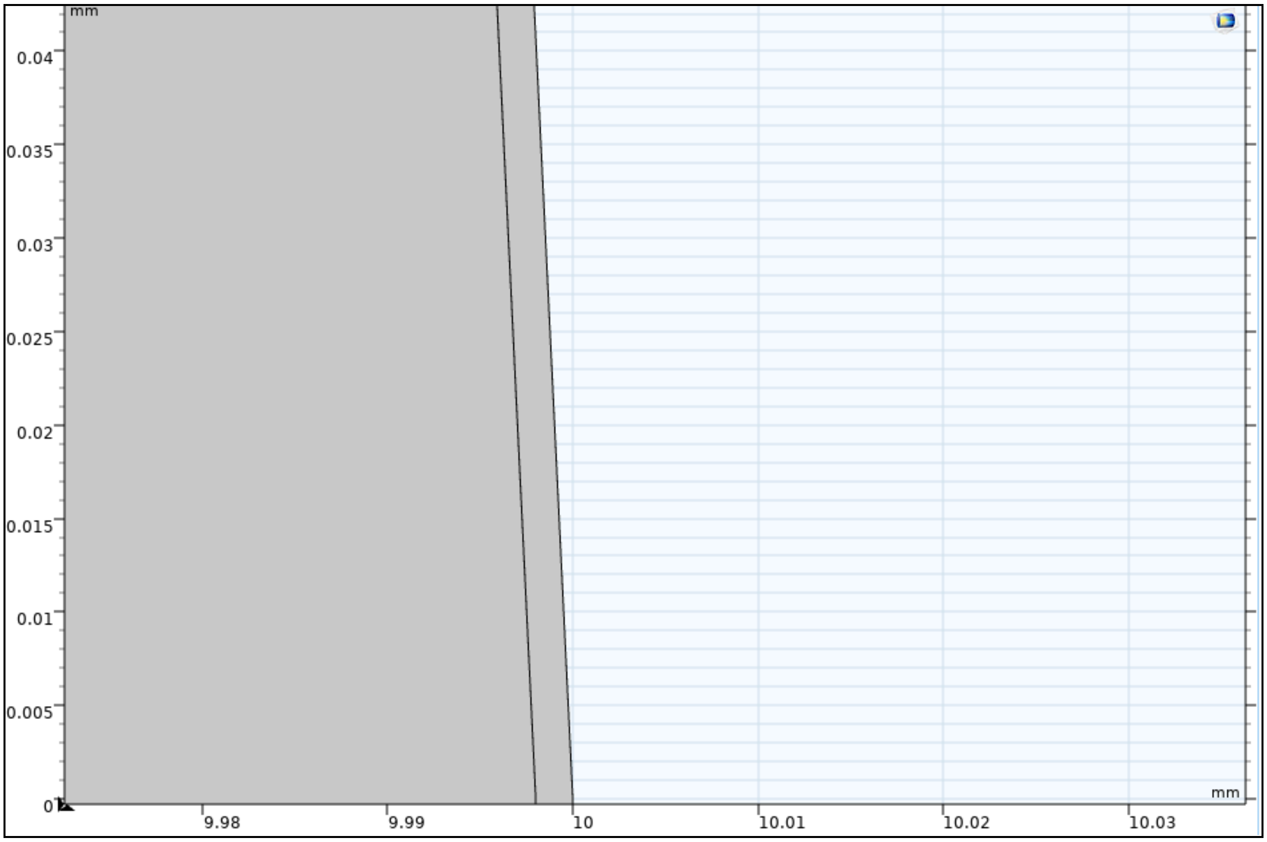

Fig 5: *Zoomed-in view of grape skin.* The skin radius was 0.002 mm and the pulp was 9.998 mm.

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Through a mesh convergence test, we determined that the simplest mesh option, extremely coarse mesh, performed as sufficiently well as more complex meshes in a shorter amount of time. Figure 6 below shows what our mesh looks like before the simulation begins. When investigating different temperature effects, we gave the mesh a shrinking velocity to account for the change in volume due to moisture loss, as shown in Equation 4 below. However, shrinkage was not applied when investigating skin diffusivity for the sake of simplicity. COMSOL's parametric sweep feature was used to simulate drying with different diffusivities, while separate singular simulations were used when investigating temperature.

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$$v_{mesh} = \frac{flux\ [\frac{kg}{m^2 * s}]}{\rho\ [\frac{kg}{m^3}]}$$

Equ 4: *Mesh velocity equation.* COMSOL provided a variable for the outward moisture flux during the simulation, and we divided by the density of water to obtain a shrinkage velocity. COMSOL correctly applies this shrinkage uniformly around the grape.

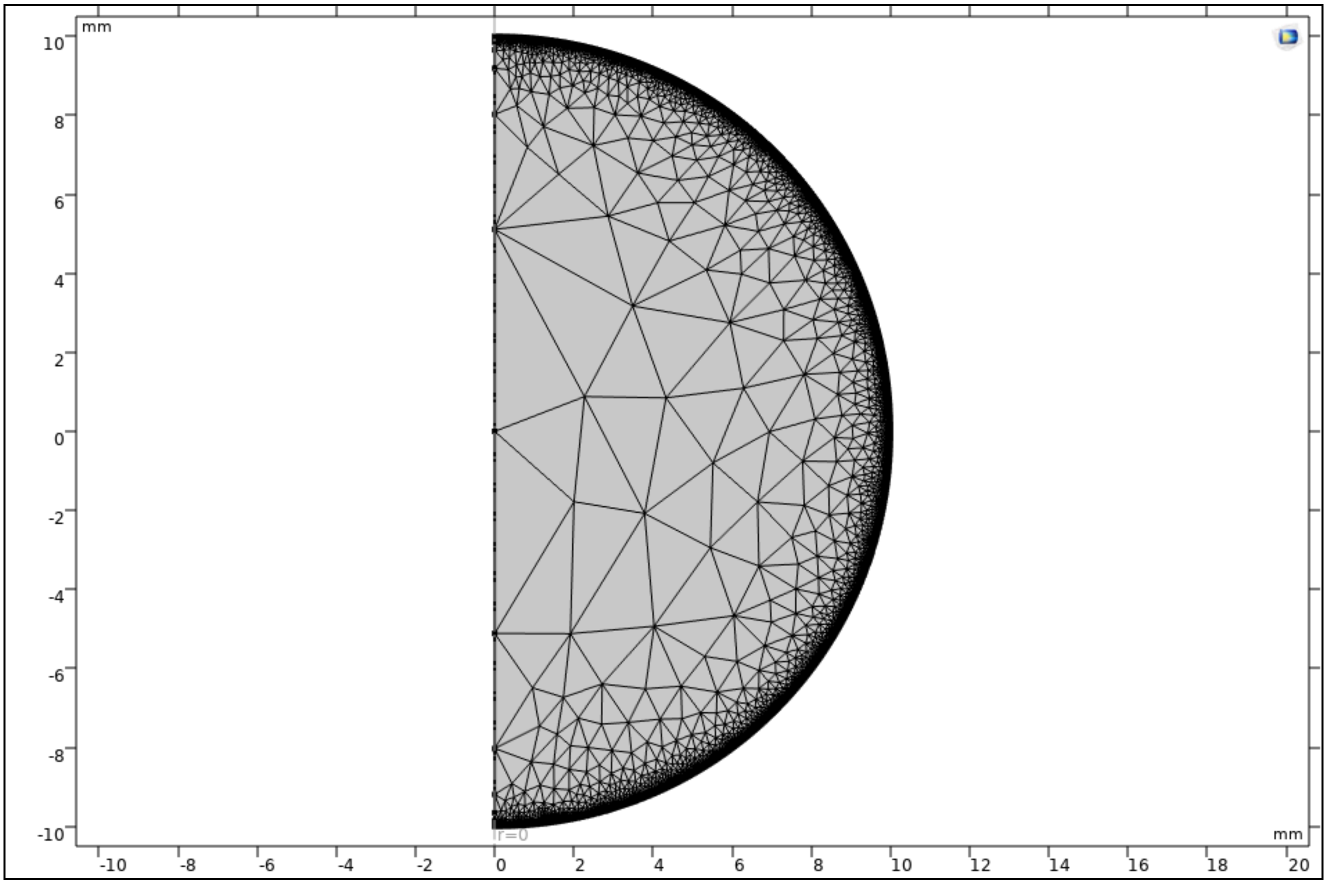

Fig 6: *Extremely coarse mesh at beginning of simulation.* This mesh option performed as sufficiently well as more complex meshes in a shorter amount of time.

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4. Results and Discussion

4.1 Skin Diffusivity

Figure 7 below shows the simulated grape moisture content in mol/m^3 versus drying time in hours at thirteen different magnitudes of skin diffusivity that reflect untreated to highly pretreated grapes. A grape can be considered a raisin when it reaches 5-8% average moisture content, which correlates to approximately 2500 mol/m^3 to 5000 mol/m^3 in our case (Sokac et al., 2022). As Figure 7 shows, for skin diffusivities between 1x10^{-10} m^2/s to 1x10^{-12} m^2/s, the grape became a raisin in 5 hours or less. For diffusivities at 1x10^{-13} m^2/s and above, drying continued indefinitely without reaching desired levels. At diffusivities above 1x10^{-15} m^2/s, no change in moisture content occurred. These results suggest that pretreatment of grape skin is a necessary step in the grape drying process, and that an optimal range of skin diffusivity values might exist between 1×10^{-10} m^2/s to 1×10^{-12} m^2/s. This aligns with the current literature on grape drying (Adiletta et al., 2016; Saravacos et al., 2001, Sokac et al., 2022).

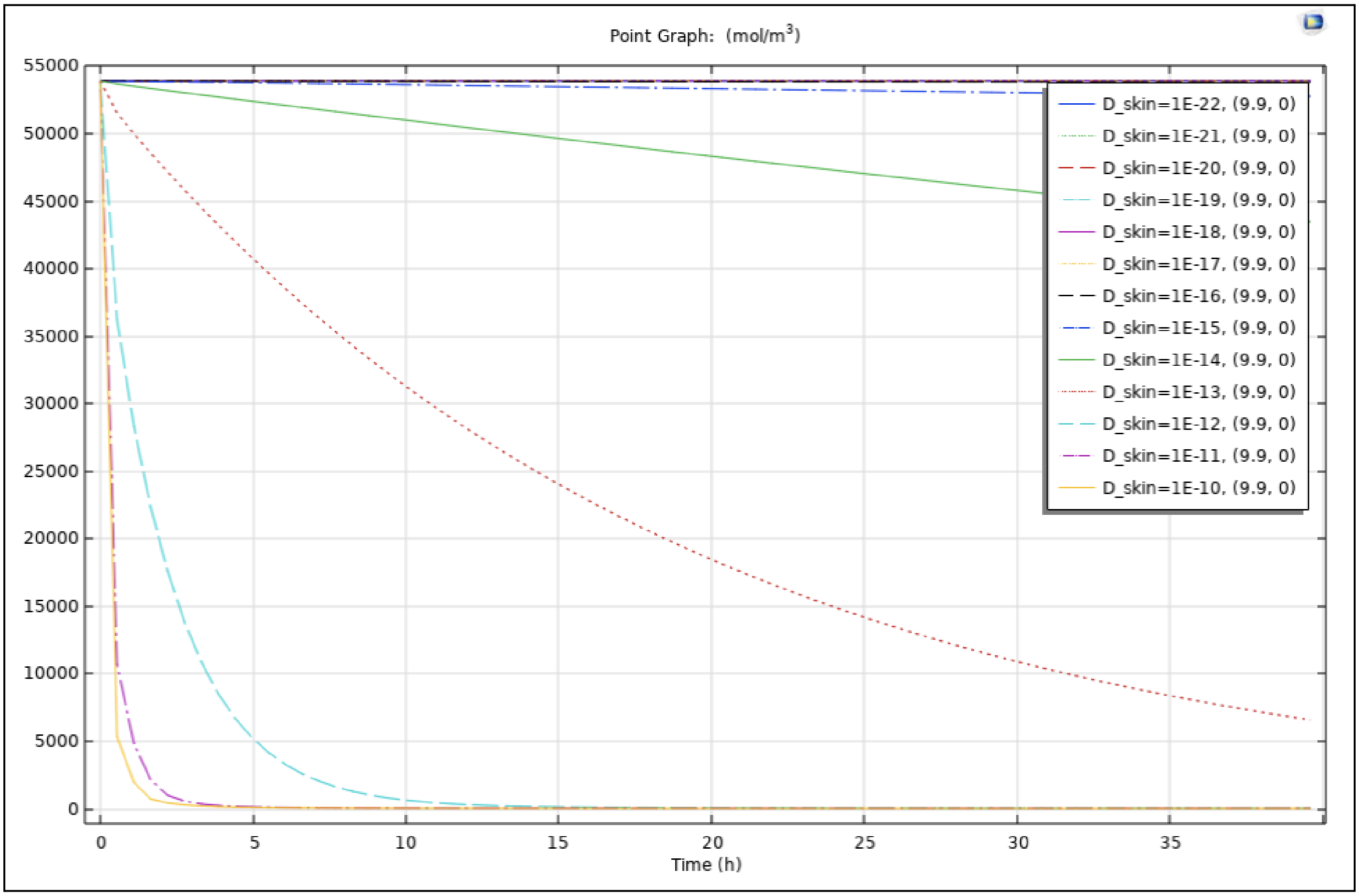

Figure 7: *Parametric sweep results for grape moisture content in mol/m^3 vs drying time in hours at different skin diffusivities.* A grape is considered a raisin at 5-8% moisture content, or roughly 2500 mol/m^3 to 5000 mol/m^3 in our case. Diffusivities above 1×10^{-12} m^2/s resulted in unreasonable drying times well beyond 35 hours. The highest diffusivities resulted in no change in moisture content.

4.2 Temperature

Table 1a below shows the isobaric vacuum drying time for grapes at different temperatures from Sokac et al., 2022. Our simulation results under the same external conditions with a skin diffusivity of 1×10^{-10} m^2/s are shown in Table 1b, which disagrees with the exact times Sokac et al. but agrees with the trend that increased temperature decreases drying time. At 35°C, our simulation was unable to finish running and crashed for unknown reasons at 6.45 hours with a

28.9% moisture content. At five and three hours, our simulation finished but did not reach the desired 5-8% moisture content. Table 1c below shows how long our model could run until crashing at the different temperatures, and what the resulting moisture content was. At 50°C and 70°C, we were able to reach desired moisture content levels after longer times than the researchers. Figure 8 below shows a .gif of the spatial moisture distribution through five hours of drying with a temperature of 50°C and a skin diffusivity of $1x10^{-10}$ m^2/s

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(1a)

Drying Process	Temperature (°C)	Pressure	Drying Time (h)
Vacuum drying	35	100 mbar	12
Vacuum drying	50	100 mbar	5
Vacuum drying	70	100 mbar	3

(1b)

Temperature (C)	Time Run (h)	Moisture Content (%)
35	6.45*	28.9
50	5	57.2
70	3	59.0

(1c)

Temperature (C)	Max Time Ran (hr)	Moisture Content (%)
35	6.45	28.9
50	8.11	6.12
70	7.89	3.87

Table 1a/b/c: *Simulation results compared to literature results from Sokac et al., 2022.* **(1a)** shows the external conditions and resulting drying time for grapes from the researchers. **(1b)** shows our results under the same conditions. The simulation was unable to finish running for unknown reasons at 35°C, and was unable to meet the desired 5-8% moisture content at 50°C and 70°C. **(1c)** shows how long the simulation was able to run until crashing and the resulting moisture content. At 50°C and 70°C we were able to reach the desired 5-8% moisture content.

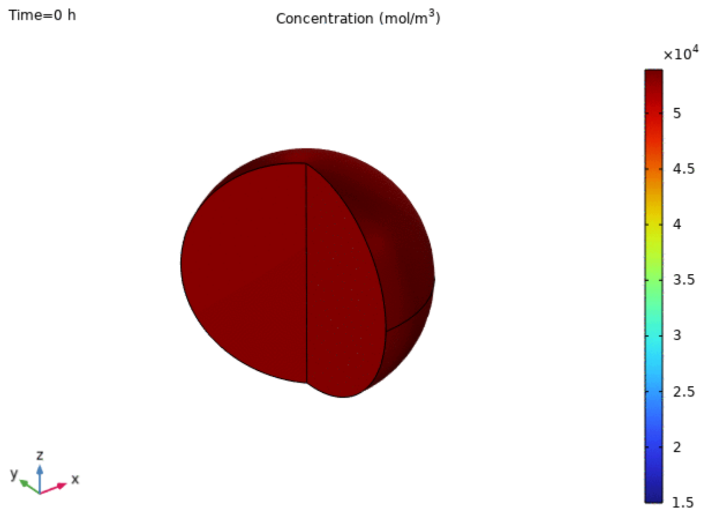

Figure 8: *Spatial moisture distribution.* This .gif shows the spatial moisture distribution through five hours of drying with a temperature of 50°C and a skin diffusivity of 1×10^{-10} m^2/s. This correlates to the scenario in Table 1b, row 2.

To investigate these disagreements in results, we first critiqued our own model's validity. Figure 9 below shows a comparison of how we simulated shrinkage versus a model from Simal et al., 1996. The root mean square error between the radii was calculated as 0.399 mm, indicating a high similarity between our simulation and the model from the researchers.

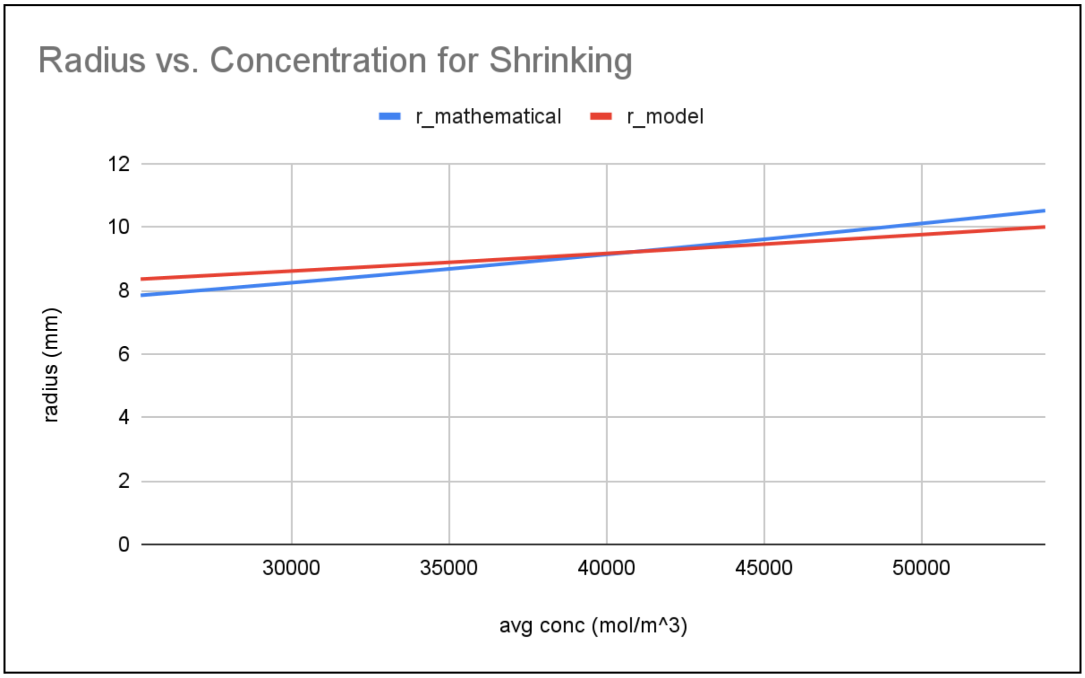

Fig 9: *Comparison of radii due to shrinkage for our simulation versus a model from Simal et al., 1996.* The researchers found a linear relationship of $V_{grape}/V_{initial} = 0.2276 + 0.2151*W$, where W is the average grape moisture content. This equation was rearranged for the grape radius and compared with our radius during shrinkage. We calculated a 0.399 mm root mean square error between our radii and that of the researchers' model. This indicates an accurate simulation of shrinkage.

Due to limited class time, we were unable to investigate the causes of these different results any further. We would have first liked to do a deeper dive into other literature to see if there were studies or simulations that agreed with our results, or if there were other conditional factors that could explain our differences. From there, we would have liked to refine our simulation, given the fact it inexplicably crashed early in the scenario at 35°C. All input values, equations, and COMSOL settings would be reevaluated given more time. Beyond this, we would look closer at our problem setup and assumptions. For example, an assumption we would have reconsidered is that the grape moisture was entirely in the liquid phase and that no vapor was present. While this alone is inconsistent with mass transfer principles taught in class, it is particularly important to assess in the case of vacuum drying. This is because the low pressure in a vacuum dryer decreases the boiling temperature of water, potentially resulting in more vapor in the pores and therefore faster moisture diffusion (Clary et al., 2007). Another possibly problematic assumption was that the moisture is lost uniformly around the entire grape surface. In an actual vacuum dryer, the grapes will sit on a surface and have a portion of their outer boundary covered, resulting in nonuniform moisture loss.

5. Conclusions and Future Research

Our simulation results agree with the current literature on the effects that grape skin diffusivity has on drying times and suggest the existence of an optimal skin diffusivity range for drying between $1x10^{-10}$ m^2/s and $1x10^{-12}$ m^2/s. Knowing the minimal amount of pretreatment required for optimal results could help raisin producers save money and effort. Our simulation results agreed with the reported literature trend that increasing drying temperature decreases drying time, however, we did not find the same times. This calls into question the validity of our congruent diffusivity results, as well. Future simulations should resolve some of our simplifying assumptions to increase model accuracy and look closer at literature results.

Beyond our scope of considerations, it could be valuable to simulate how pressure affects the drying process, as well. Ideally, raisin producers would want to know the combination of maximum pressure, minimum temperature, and minimum pretreatment required to vacuum dry grapes in the most efficient manner possible. Also, many vacuum dryers incorporate microwave heating elements, whereas we only simulated convective (Clary et al., 2007). COMSOL is capable of simulating microwave heating, and this could provide valuable insight into the drying process. All future simulation results should be verified in real experiments.

6. References

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