## APPENDIX: app for scale up in rotary calciners

### Access

The app for heat transfer in rotary calciners is available at pharmahub.org. Registration is required to access the tool (register at <u>https://pharmahub.org/register</u>). In addition to registration, membership to the 'calcinationgroup' group on the pharmahub is required to use the tool. Once you register at pharmahub.org, you can request membership for the 'calcinationgroup' at <u>https://pharmahub.org/groups/calcinationgroup</u> (or contact Dr. Bereket Yohannes email: <u>bereket.yohannes@rutgers.edu</u> to be added to the group).

Once the registration is complete and group membership is granted, you can access the app at <u>pharmahub.org</u>. Figure A1 shows how to access the app at <u>pharmahub.org</u>. Follow the three steps shown in the figure to access the tool.



## 1. https://pharmahub.org/resources/tools

Figure A1. Accessing the SURC tool on pharmahub.org

### Brief user manual

The app can be run with or without axial velocity of powder bed. Figure A2-A9 show the most important components of the app. C*lick the 'OK' button to run the simulation* (Fig. A2). For all runs the relationship between the timescales and the evolution of the minimum, average, and maximum temperatures are plotted. In addition, the values of the temperatures are listed in a table form.

The types of analysis that can be done using the app are presented step by step in this appendix.

# 1. To study the relationship between timescales using the scale up equation shown in Eq. 8 in the main report. (Level I run)

The inputs are only  $\phi$ , fill area, particle size, wall temperature, and initial temperature. Based on these inputs,  $\tau$  and the temperature profile are computed. (Fig. A2).



Figure A.2: Level I run. Inputs are the dimensionless parameter  $\phi$ , fill Area A, particle size d, wall temperature  $T_w$  and initial temperature  $T_o$ . The cross-section area  $A_p$  and the thermal time  $\tau$  are computed. All computed variable are highlighted in yellow.

## To study the effect of operating conditions (diameter of calciner, speed of rotation, and fill level) on the thermal time parameter τ. (Level II run)

Inputs include operating conditions (fill angle ( $\theta$ ), speed of rotation ( $\omega$ ), and calciner diameter (D)). From these inputs,  $\tau_c$  is computed.  $\tau_p$  is directly read from the GUI ( $\tau_p$  is not computed for this level). Then,  $\phi$  will be computed as the ratio of  $\tau_p$  and  $\tau_c$ . (Fig. A3). Note that the operating conditions box is checked.



Figure A.3: Level II run. Inputs are particle size d, wall temperature  $T_w$  and initial temperature  $T_o$  speed of rotation  $\omega$ , drum size D, the fill level (% or fill angle  $\theta$ ), and the time to heat one particle  $\tau_p$ . The outputs are the thermal time  $\tau$ ,  $\phi$ , contact time  $\tau_c$ , cross-section area  $A_p$  and the fill area A. The axial velocity is ignored. All computed variable are highlighted in yellow.

## To study the effect of particle thermal and mechanical properties on the thermal time parameter τ. (Level III run).

In Level II run,  $\tau_c$  was a user defined input. In level II run,  $\tau_c$  is computed from the thermal and mechanical properties of the particles (Fig. A4). Note that the material properties box is checked.



Figure A.4: Level III run. Inputs are particle size d, wall temperature  $T_w$  and initial temperature  $T_o$ , speed of rotation  $\omega$ , drum size D, the fill level (% or fill angle  $\theta$ ), particle density  $\rho$ , thermal conductivity k, heat capacity  $c_p$ , modulus of elasticity E, and Poisson's ratio v. The outputs are the thermal time  $\tau$ ,  $\phi$ , contact time  $\tau_c$ , time to heat one particle  $\tau_p$ , cross-section area  $A_p$  and the fill area A. The axial velocity is ignored. All computed variable are highlighted in yellow.

### 4. Include the axial velocity of the powder bed directly. Level IV run.

In Level I-III runs, the temperature profile is computed as a function of time. In level IV run the temperature profile is plotted as function of distance from inlet. This type of analysis can assist in predicting the length of calciner required for the process. In this run, the axial velocity u is defined by the user directly. The plug flow choice is selected from the drop down menu and the value of u is input. (Fig. A5)



Figure A.5: Level IV run. The basic inputs are particle size d, wall temperature  $T_w$  and initial temperature  $T_o$ , speed of rotation  $\omega$ , drum size D, and the fill level (% or fill angle  $\theta$ ). In addition, the user can opt to define the  $\tau_p$  directly or compute  $\tau_p$  by inputting particle density  $\rho$ , thermal conductivity k, heat capacity  $c_p$ , modulus of elasticity E, and Poisson's ratio  $\nu$  The outputs are the thermal time  $\tau$ ,  $\phi$ , contact time  $\tau_c$ , time to heat one particle  $\tau_p$ , cross-section area  $A_p$  and the fill area A. Note that the temperature profile is plotted as function of distance *l* from the inlet. In this case, when u=2m/s, the temperature of the particles reach the wall temperature at *l*=0.074m. All computed variable are highlighted in yellow.

#### 5. Compute the axial velocity using Sullivan Model (Level V run).

In Level IV runs, the axial velocity is defined directly by the user. In level V run, the axial velocity is computed based on the operating conditions and the bulk properties of the powder. The bulk properties include the coefficient of friction and bulk density of the powder bed. In addition, the feed rate and the inclination angle of calciner are inputs in level V run. (Fig. A6)



Figure A.6: Level V run. The basic inputs are particle size d, wall temperature  $T_w$  and initial temperature  $T_o$ , speed of rotation  $\omega$ , drum size D, the feed rate, incline angle, bulk density  $\rho_b$ , and bulk coefficient of friction  $\mu_b$ . In addition, the user can opt to define the  $\tau_p$  directly or compute  $\tau_p$  by inputting particle density  $\rho$ , thermal conductivity k, heat capacity  $c_p$ , modulus of elasticity E, and Poisson's ratio v The outputs are the thermal time  $\tau$ ,  $\phi$ , contact time  $\tau_c$ , time to heat one particle  $\tau_p$ , the fill level (and  $\theta$ ), cross-section area  $A_p$  and the fill area A. Note that the temperature profile is plotted as function of distance *l* from the inlet. In this example, the axial velocity was computed to be 0.0016m/s and the temperature of the particles reaches the wall temperature at *l*=3.0m. All computed variable are highlighted in yellow.