Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting material for:

Thermodynamic Insights into the Henry's Constant in Silicon Hyperthermal Oxidation for Fabricating Optical Waveguides

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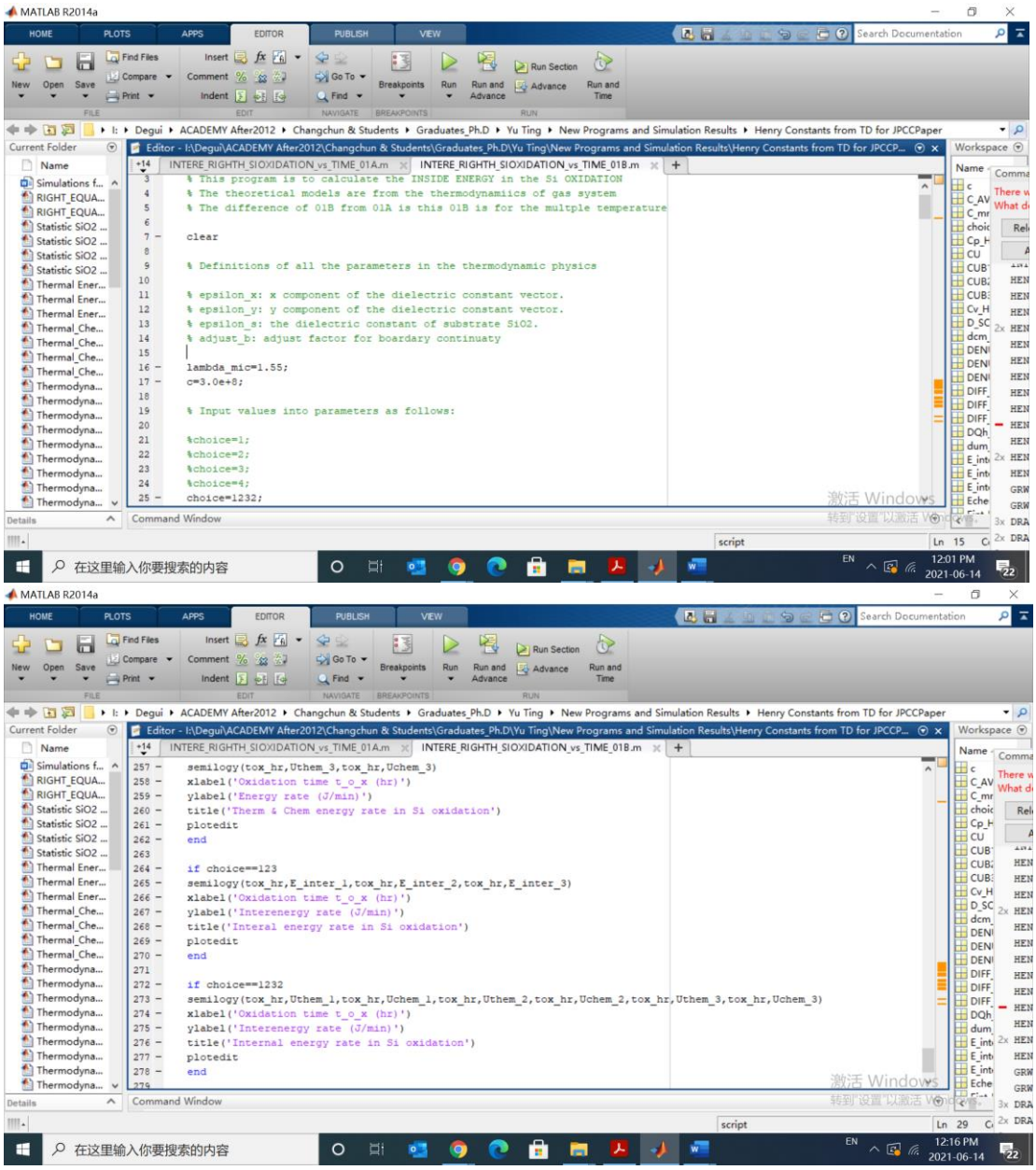
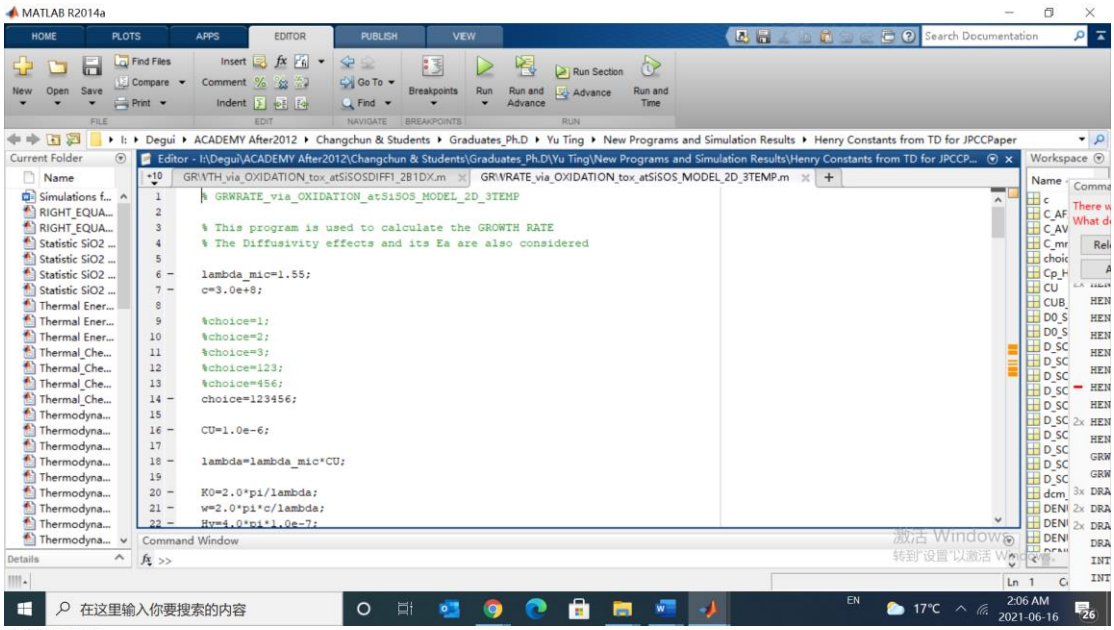
1. Thermal/chemical energies and Henry's law constant in the silicon hyperthermal oxidation system:

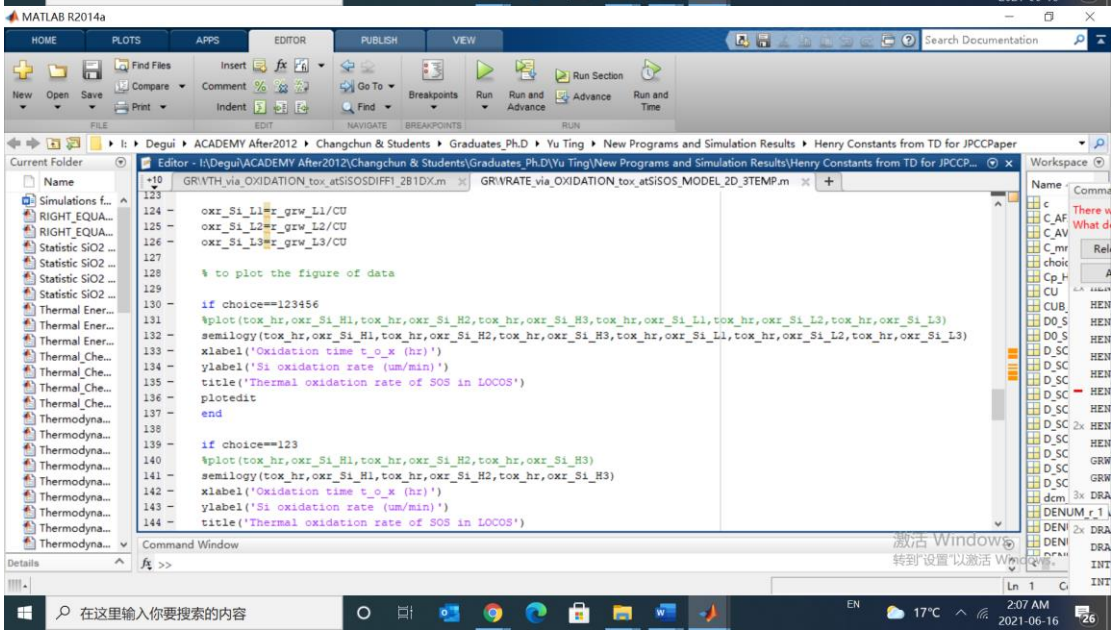
With Equations (22)-(25) in the manuscript, we use the software tool – Matlab to program and simulate the distributions of the thermodynamic and chemical reaction energies with respect to three temperature values: 700℃, 1000℃ and 1300℃ as shown in Figure 2(a), then with Equation (8) obtain the total internal energy of one molecule as shown Figure 2(b). Further, we simulate the Henry's constant H in the hyperthermal oxidation process of silicon with respect to these three temperature values as shown in Figure 3(a), then by setting an oxidation time of 1.0 h, we simulate the temperature dependence of H as shown in Figure 3(b). The follows are the start and end parts of the program.



2. Analysis for the diffusivity effect upon the Growth rate of silicon dioxide (SiO_2) in the thermodynamic mode

With the high initial diffusivity value of 8.4×10^{-7} (m^2s^{-1}), and the low initial diffusivity value 1.0×10^{-10} (m^2s^{-1}), for the three temperatures: 700℃, 1000℃ and 1300℃, with Equation (2) and the E_a effect on the diffusivity of oxidant, we obtain the simulation results of the oxidation time dependence of SiO_2 growth rate with respect to four cases as shown in Figures 4(a) and 4(b), respectively. The follows are the start and end parts of the program.

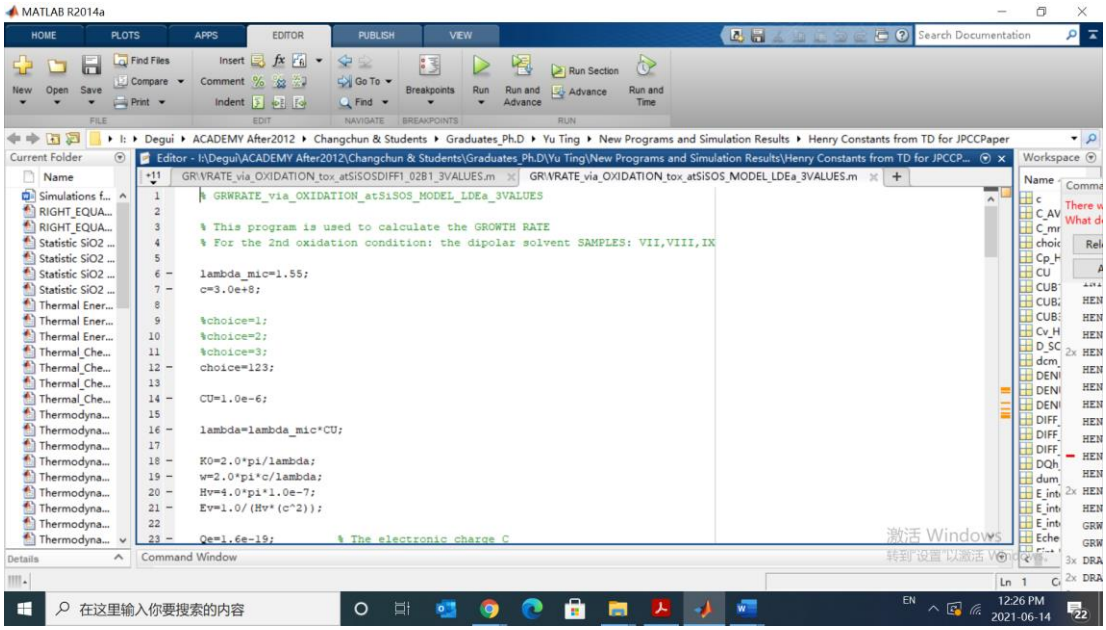


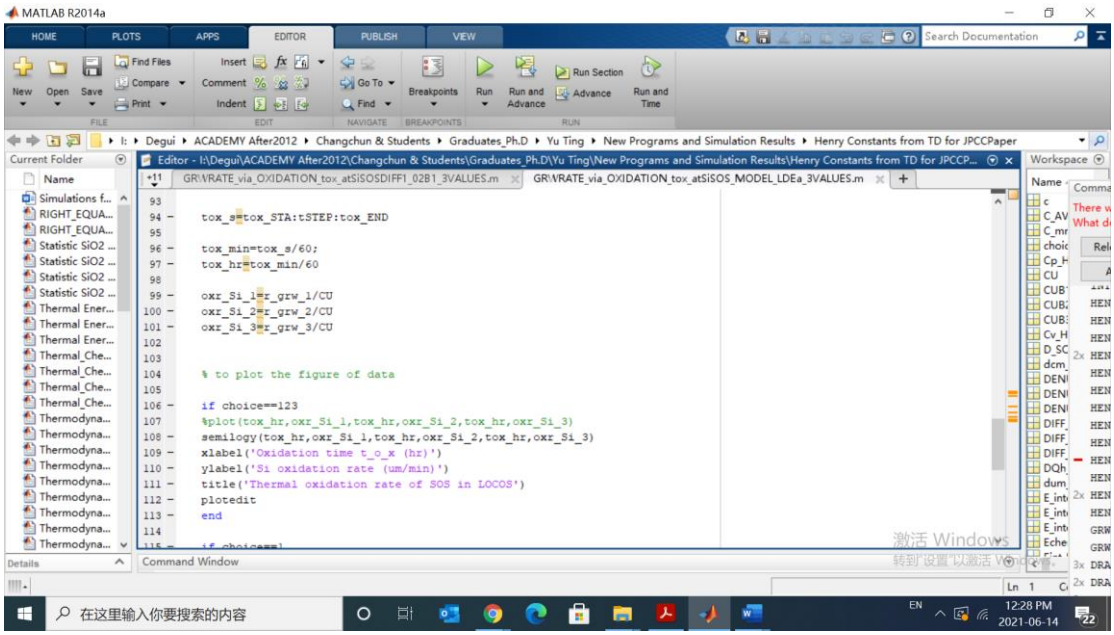


3. Growth rate of SiO_2 layer in the thermodynamic mode:

3.1. Thermodynamic Model of H with Pfeffer/Ohring's model of D:

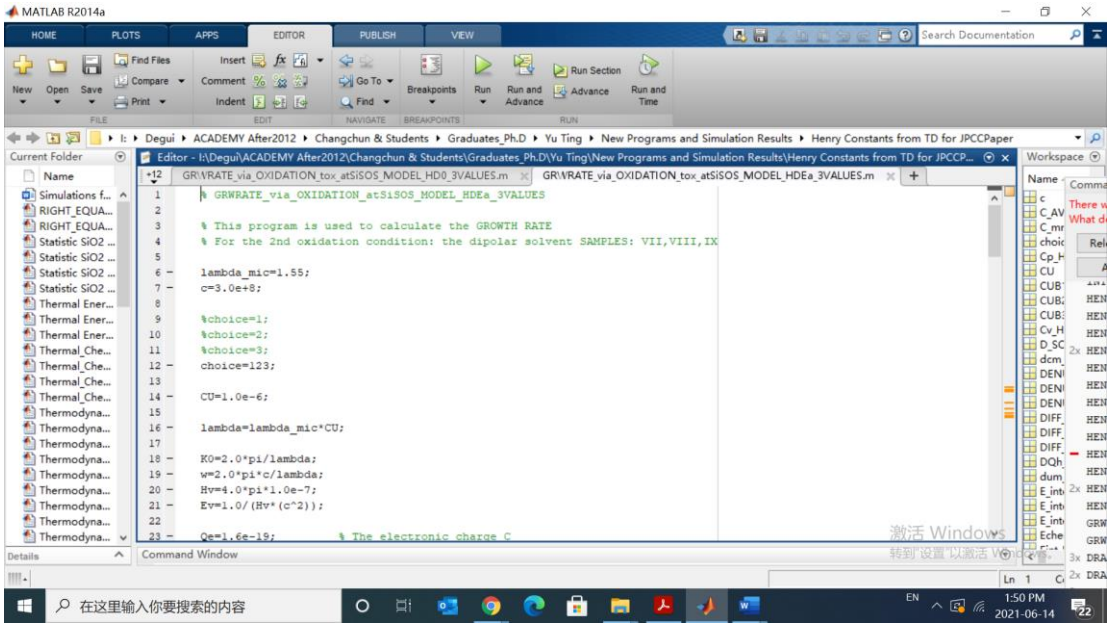
Used the following program to simulate the oxidation time dependence of SiO_2 growth rate at 21 temperatures in 700-1300℃, then obtain 21×21 matrix, then created the dual temp/time dependences of SiO_2 growth rate as shown in Figures 5(a). The follows are the start and end parts of the program.

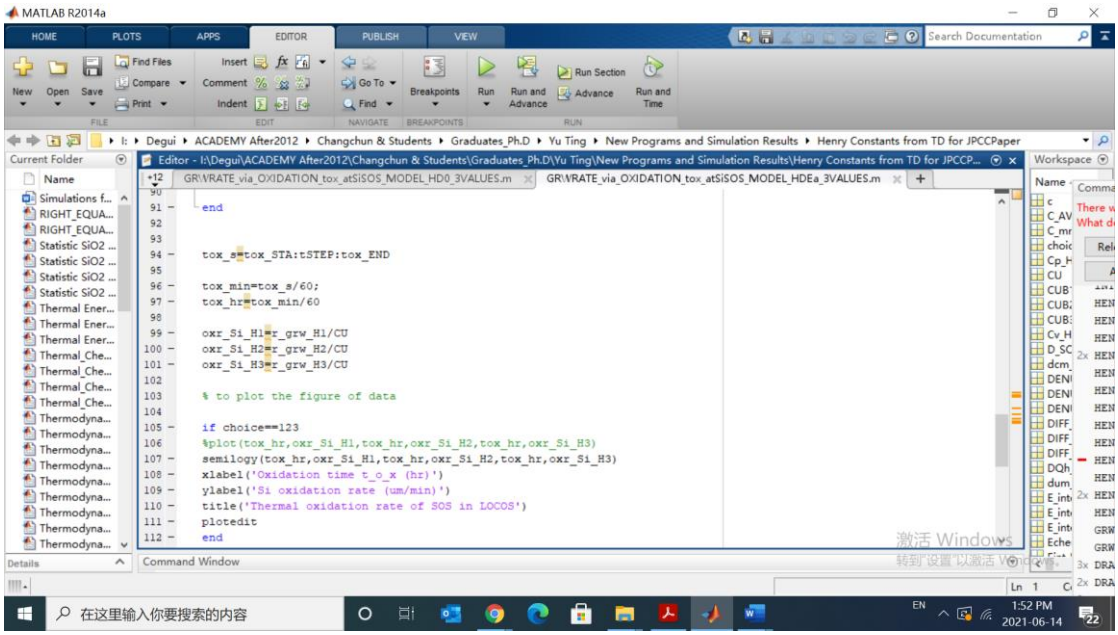




3.2. Thermodynamic Model of H with Kostinski's model of D:

Used the following program to simulate the oxidation time dependence of SiO_2 growth rate at 21 temperatures in 700-1300℃, then obtain 21×21 matrix, then created the dual temp/time dependences of SiO_2 growth rate as shown in Figures 5(b). The follows are the start and end parts of the program.

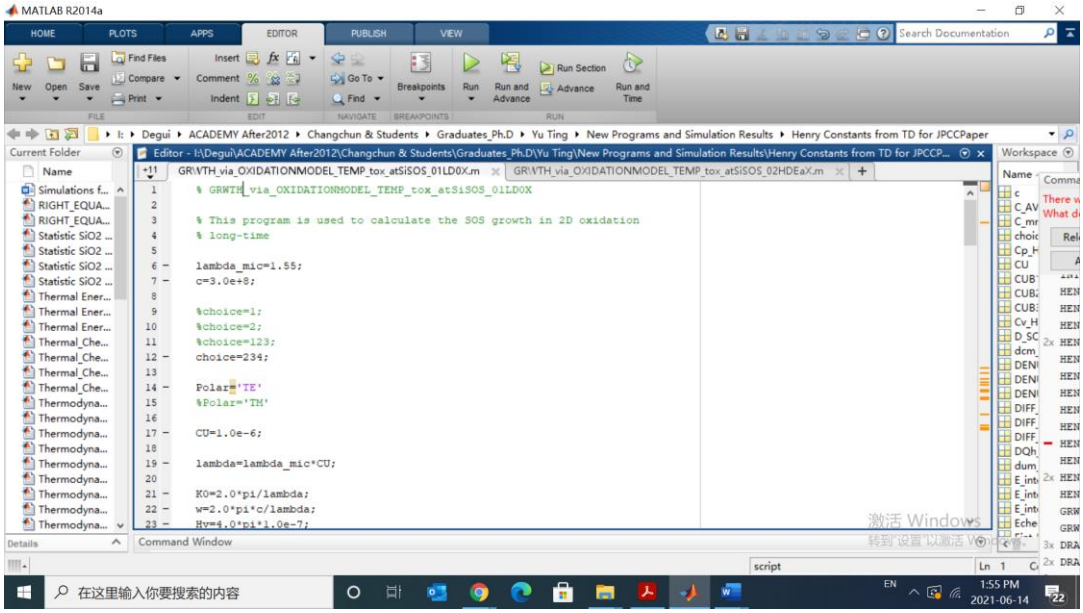


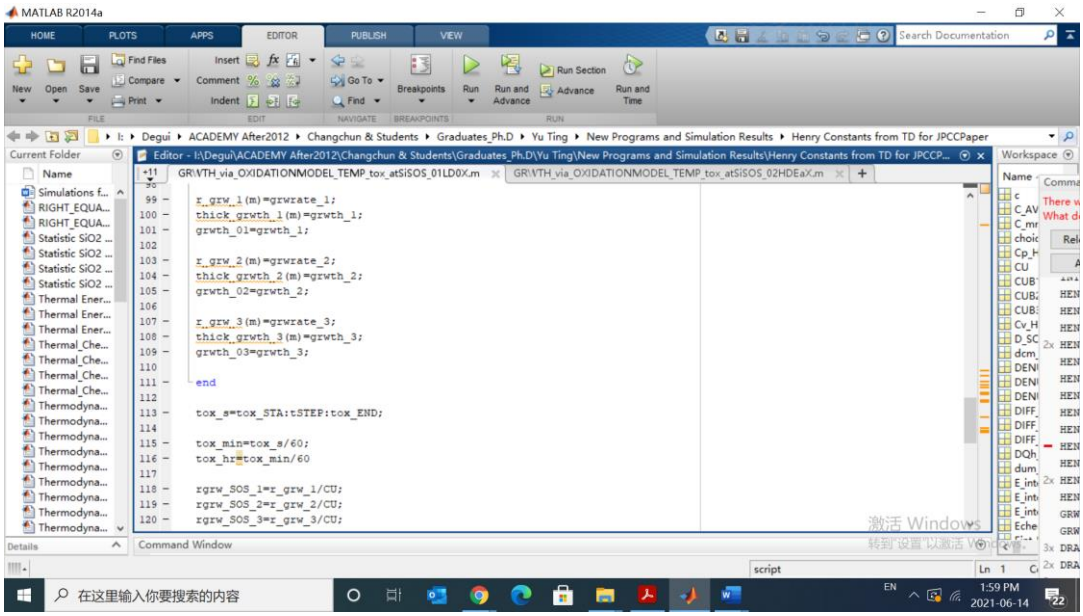


4. Thickness of SiO_2 layer in the thermodynamic mode:

4.1. Thermodynamic Model of H with Pfeffer/Ohring's model of D:

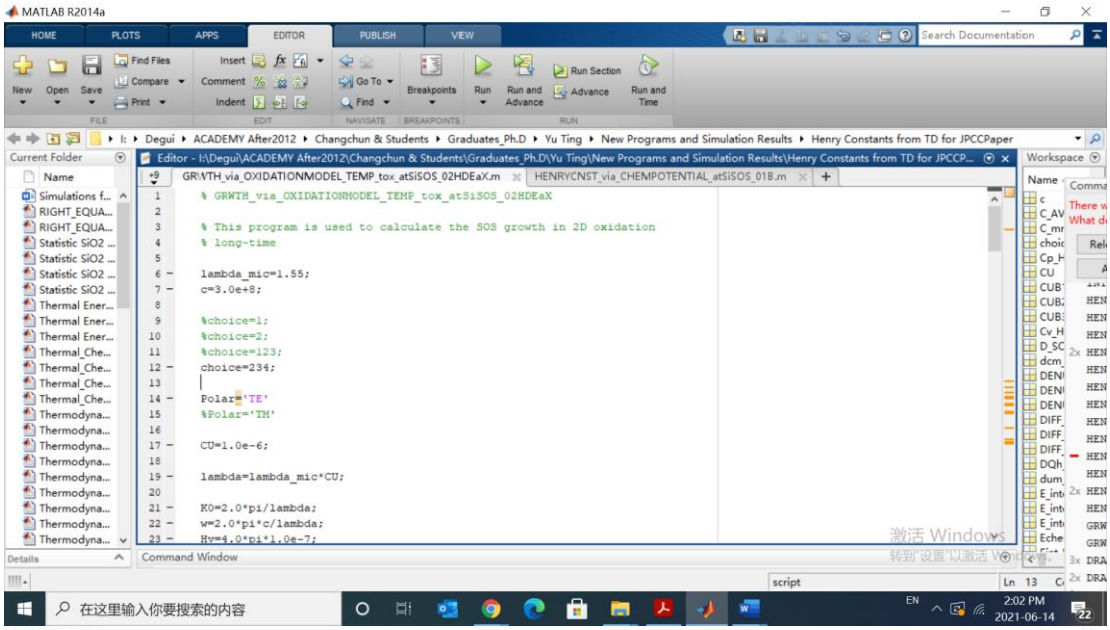
Based on simulation results for the Henry's constant and the growth rate of SiO_2 shown in Figures 3-5, by selecting the Pfeffer/Ohring's model of the diffusivity, with Equation (3), for the two cases in the above simulations, we obtain the simulation results of the 2-D dependences of the SiO_2 thickness on both the oxidation temperature and time as shown in Figures 6(a). The follows are the start and end parts of the program.

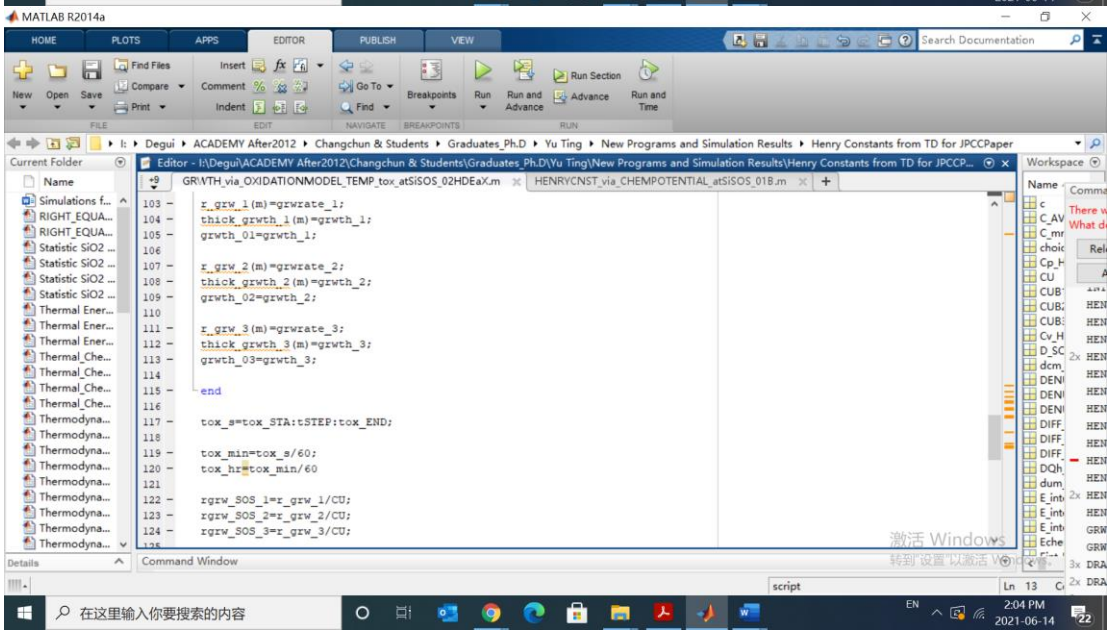




4.2. Thermodynamic Model of H with Kostinski's model of D:

Based on simulation results for the Henry's constant and the growth rate of SiO_2 shown in Figures 3-5, by selecting the Kostinski's model of the diffusivity, with Equation (3), for the two cases in the above simulations, we obtain the simulation results of the 2-D dependences of the SiO_2 thickness on both the oxidation temperature and time as shown in Figures 6(b). The follows are the start and end parts of the program.

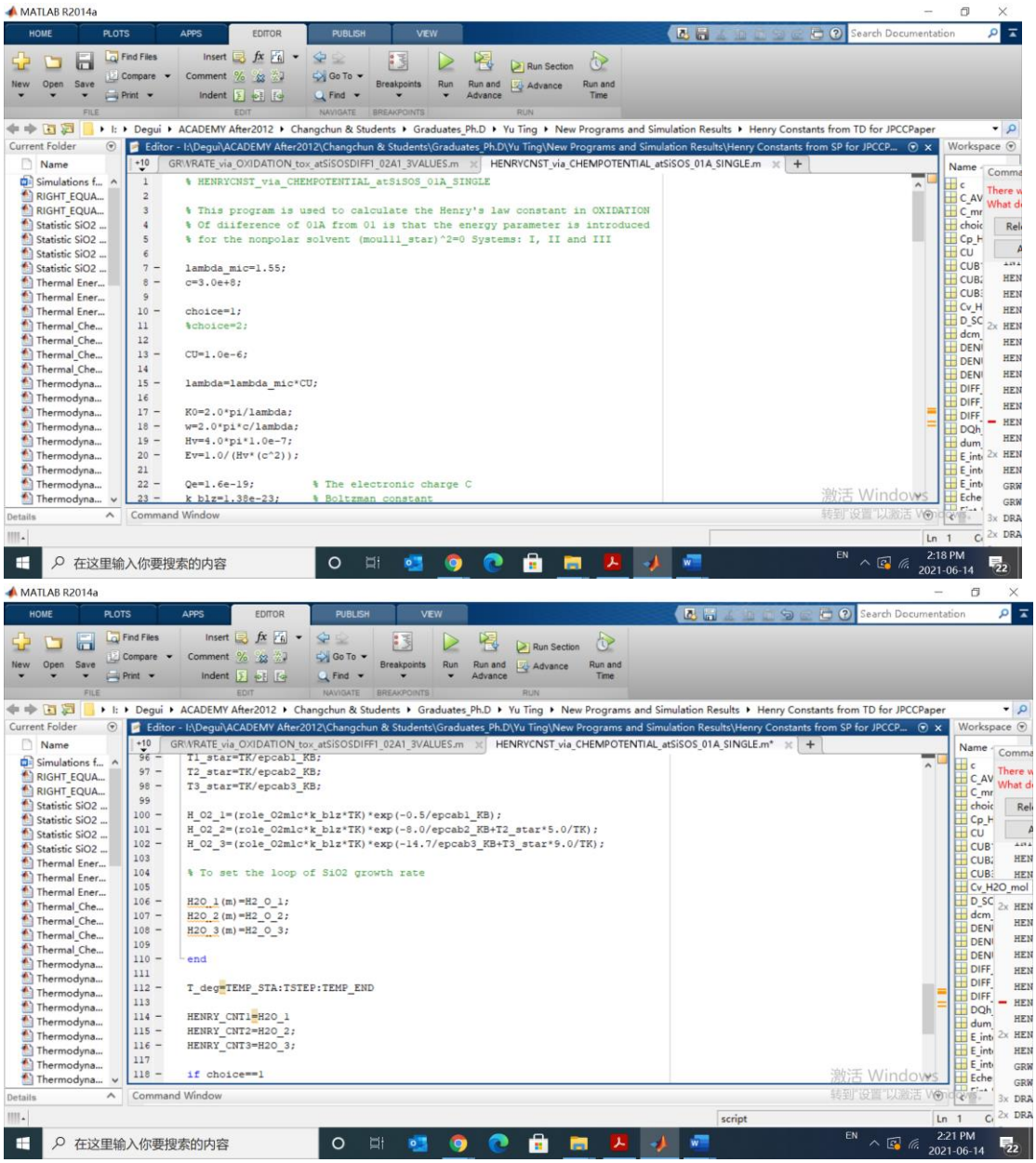




5. Henry's law constant in the empirical model:

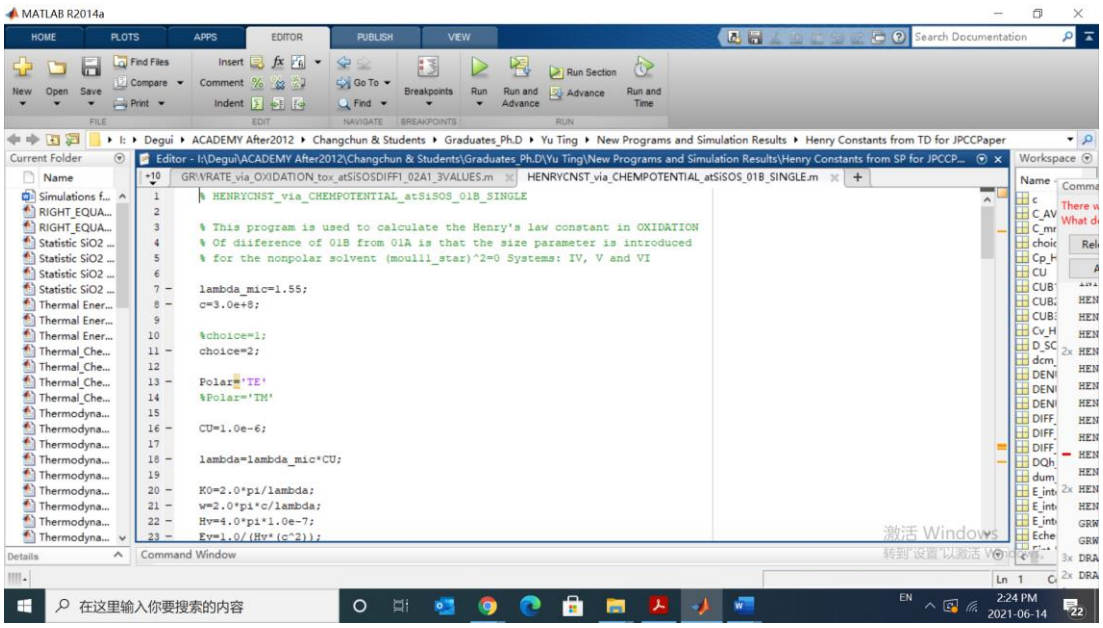
5.1. Empirical Model of H with the molecule interaction parameters: $\sigma_{ab}^{*}=1.0$, ε_{ab}^{*} has three values as 0.7071, 0.9747 and 1.2247

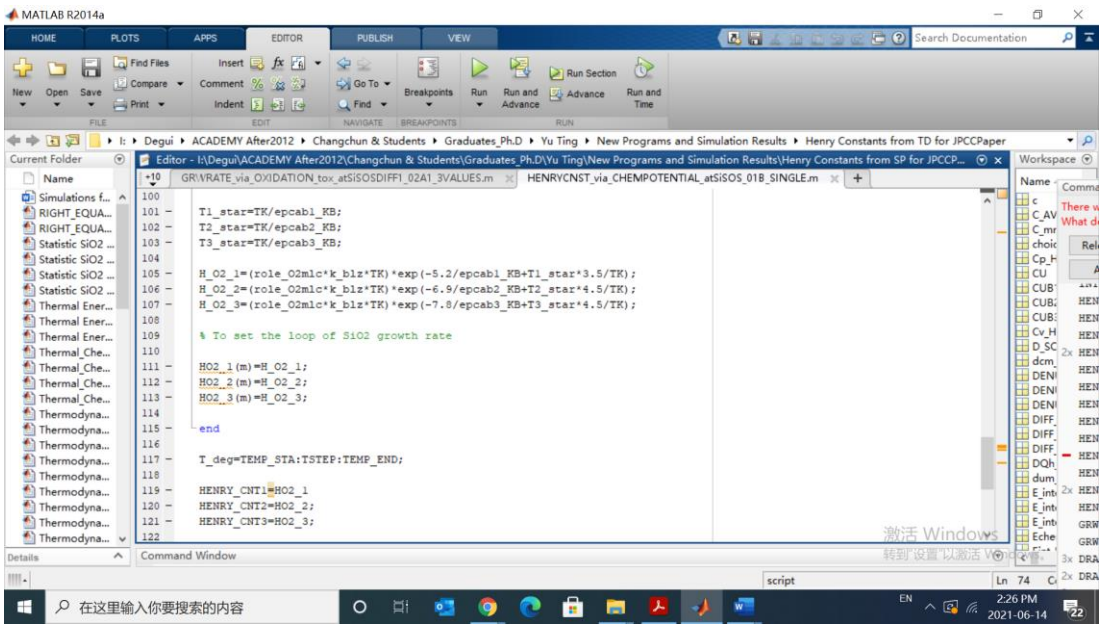
For Henry's law constant from the empirical model extracted from the published data, with Equation (7), the simulation results of Henry's constant dependences on temperature with respect to the above three values of ε_{ab}^{*} and three values of σ_{ab}^{*} as shown in Figure 7(a). The follows are the start and end parts of the program.



5.2 Empirical Model of H with the molecule interaction parameters: parameter $\varepsilon^*_{ab}=1.0$, σ^*_{ab} has three values as 0.750, 0.975 and 0.625

For Henry's law constant from the empirical model extracted from the published data, with Equation (7), the simulation results of Henry's constant dependences on temperature at ε^*_{ab}=1.0 and the three values of σ^*_{ab} as shown in Figure 7(b). The follows are the start and end parts of the program.



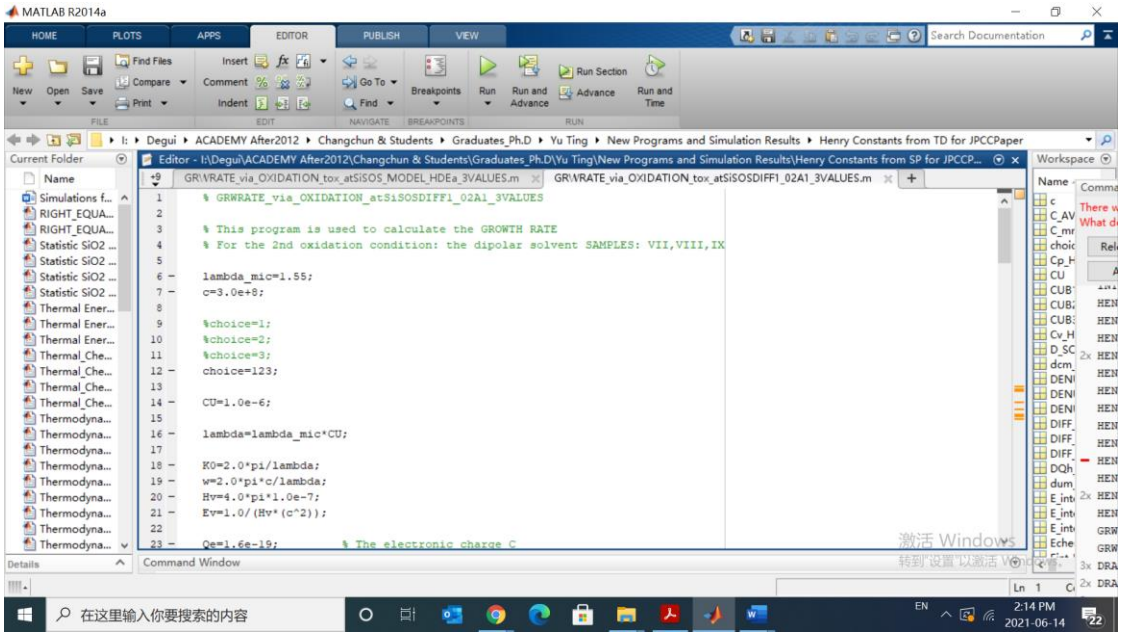


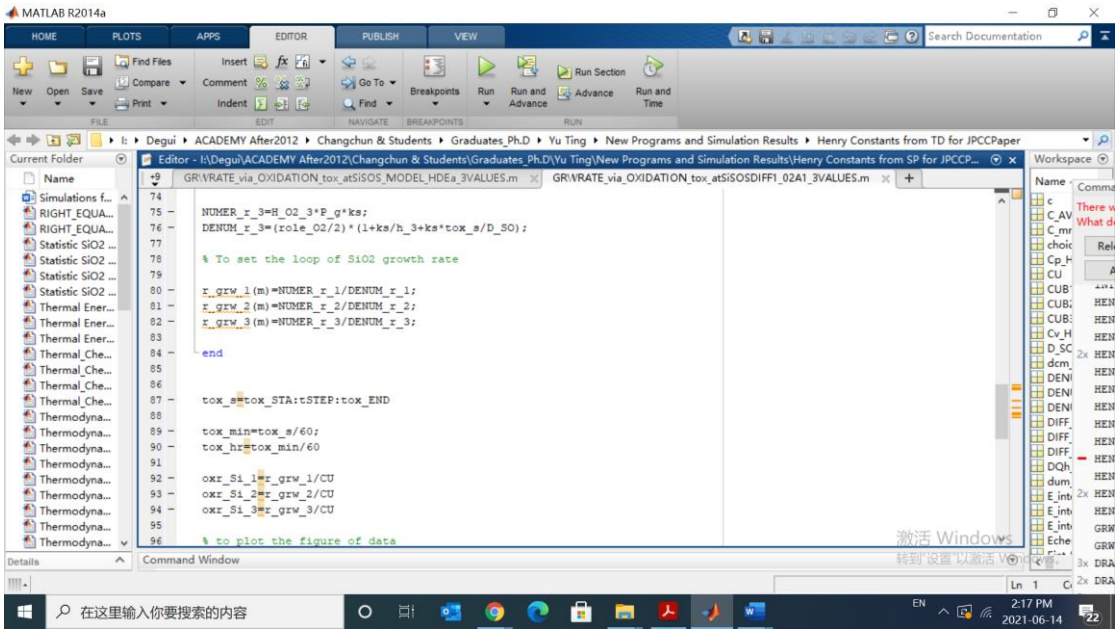
6. Growth rate of silicon dioxide (SiO_2) in the empirical mode:

6.1. Growth rate of SiO_2 with the molecule interaction parameters:

$\sigma_{ab}^{*}=1.0$, $\varepsilon_{ab}^{*}=0.7071$

For System VII, by selecting the Pfeffer/Ohring's model for the diffusivity of H_2O in SiO_2 as $D_0=1.0\times10^{-10}$ $(m^2s^{-1})/E_a=0$, with Equation (2), we simulate the thermal oxidation rates depending on both the oxidation temperature and time for these two systems as shown in Figures 8(a). The follows are the start and end parts of the program.

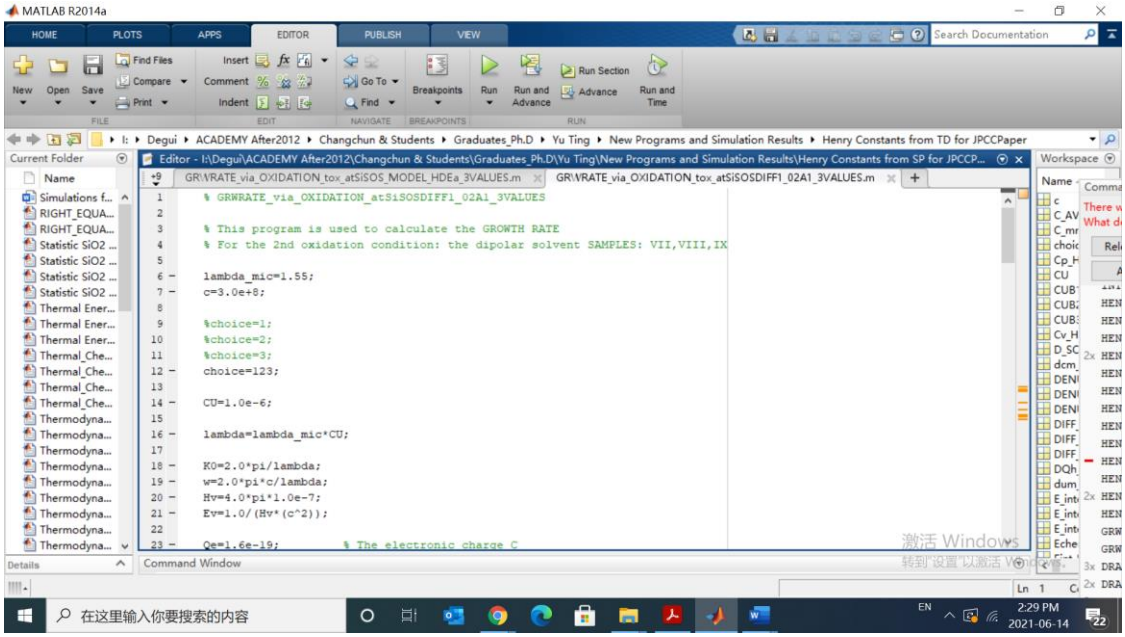


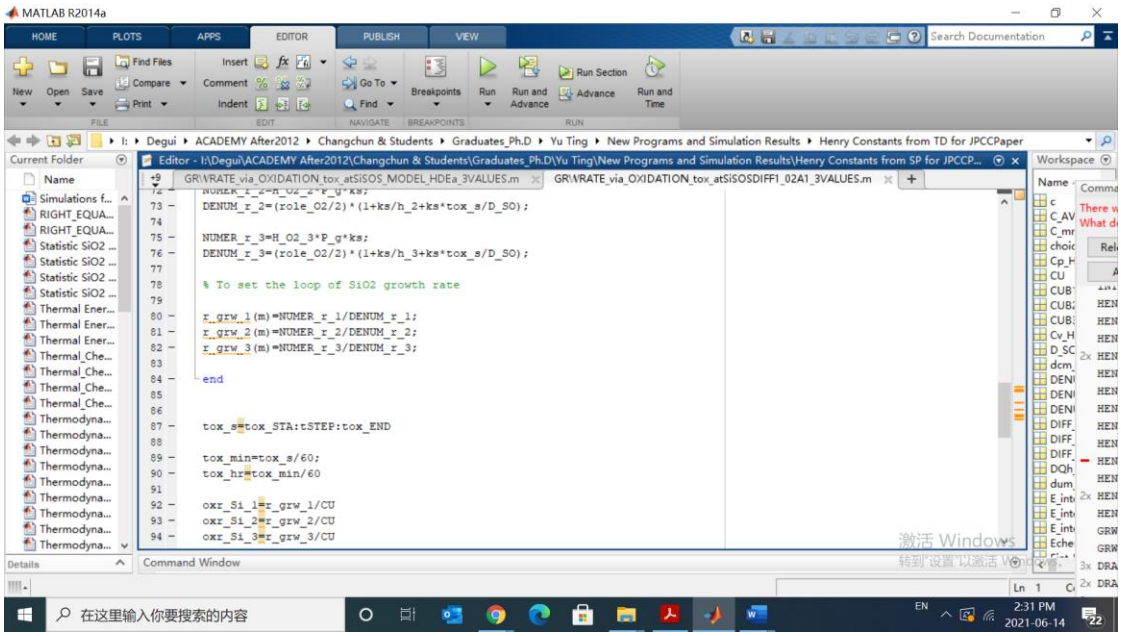


6.2 Growth rate of SiO_2 with the molecule interaction parameters:

$\varepsilon_{ab}^{*}=1.0$, $\sigma_{ab}^{*}=0.625$

For System XII, by selecting the Pfeffer/Ohring's model for the diffusivity of H_2O in SiO_2 as $D_0=1.0\times10^{-10}$ $(m^2s^{-1})/E_a=0$, with Equation (2), we simulate the thermal oxidation rates depending on both the oxidation temperature and time for these two systems as shown in Figures 8(b). The follows are the start and end parts of the program.

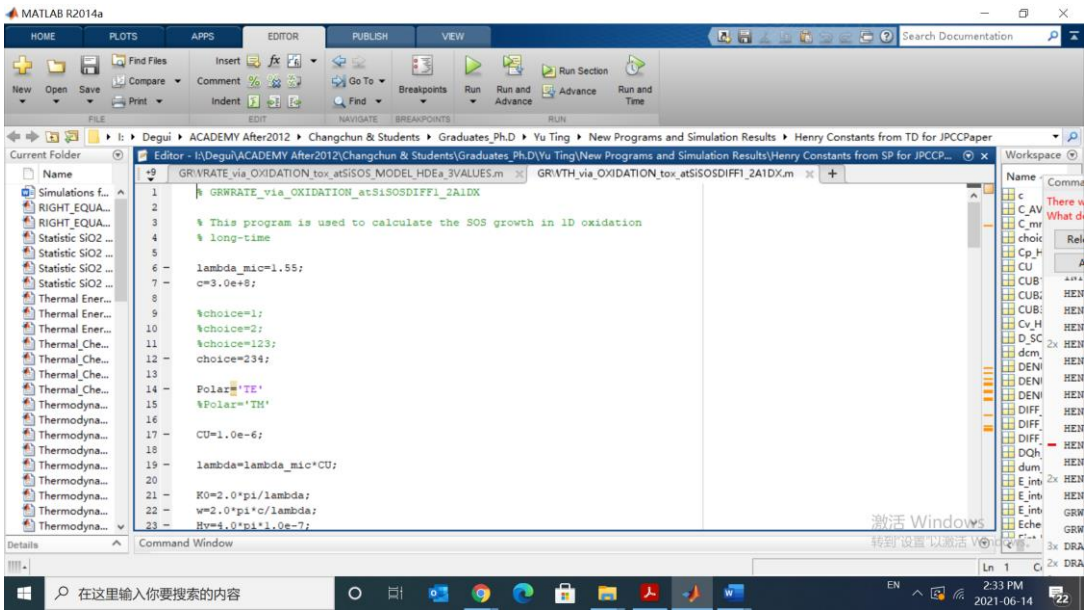


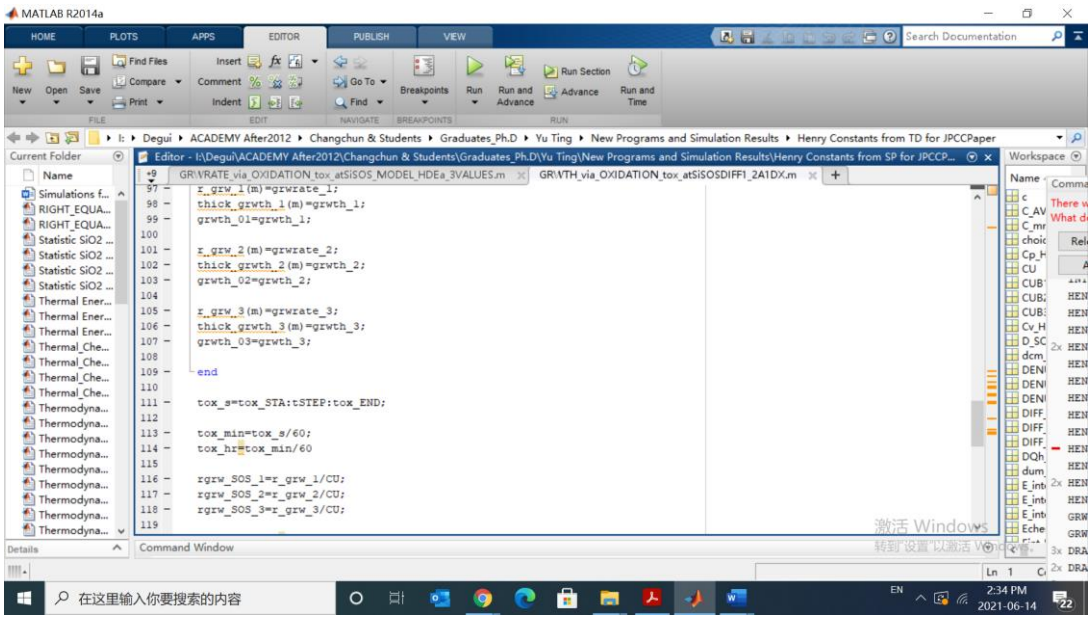


7. Thickness of SiO_2 layer in the empirical mode:

7.1. Molecule interaction parameters: $\sigma_{ab}^{*}=1.0$, $\varepsilon_{ab}^{*}=0.7071$

For System VII, by selecting the Pfeffer/Ohring's model for the diffusivity of H_2O in SiO_2 as $D_0=1.0\times10^{-10}$ $(m^2s^{-1})/E_a=0$, with Equation (3) and the same values of parameters as used in the above simulations of silicon oxidation rates, we obtain the simulation results of the 2-D dependences of SiO_2 thickness of System: VII as shown in Figure 9(a). The follows are the start and end parts of the program.





7.2 Molecule interaction parameters: $\varepsilon^*_{ab} = 1.0$, $\sigma^*_{ab} = 0.625$

For System XII, by selecting the Pfeffer/Ohring's model for the diffusivity of H_2O in SiO_2 as $D_0 = 1.0\times10^{-10}$ $(m^2s^{-1})/E_a = 0$, with Equation (3) and the same values of parameters as used in the above simulations of silicon oxidation rates, we obtain the simulation results of the 2-D dependences of SiO_2 thickness of System: XII as shown in Figure 9(b). The follows are the start and end parts of the program.