

APPENDIX B

Program Developed in This Work

Simulation of Polymer Crystallization Program

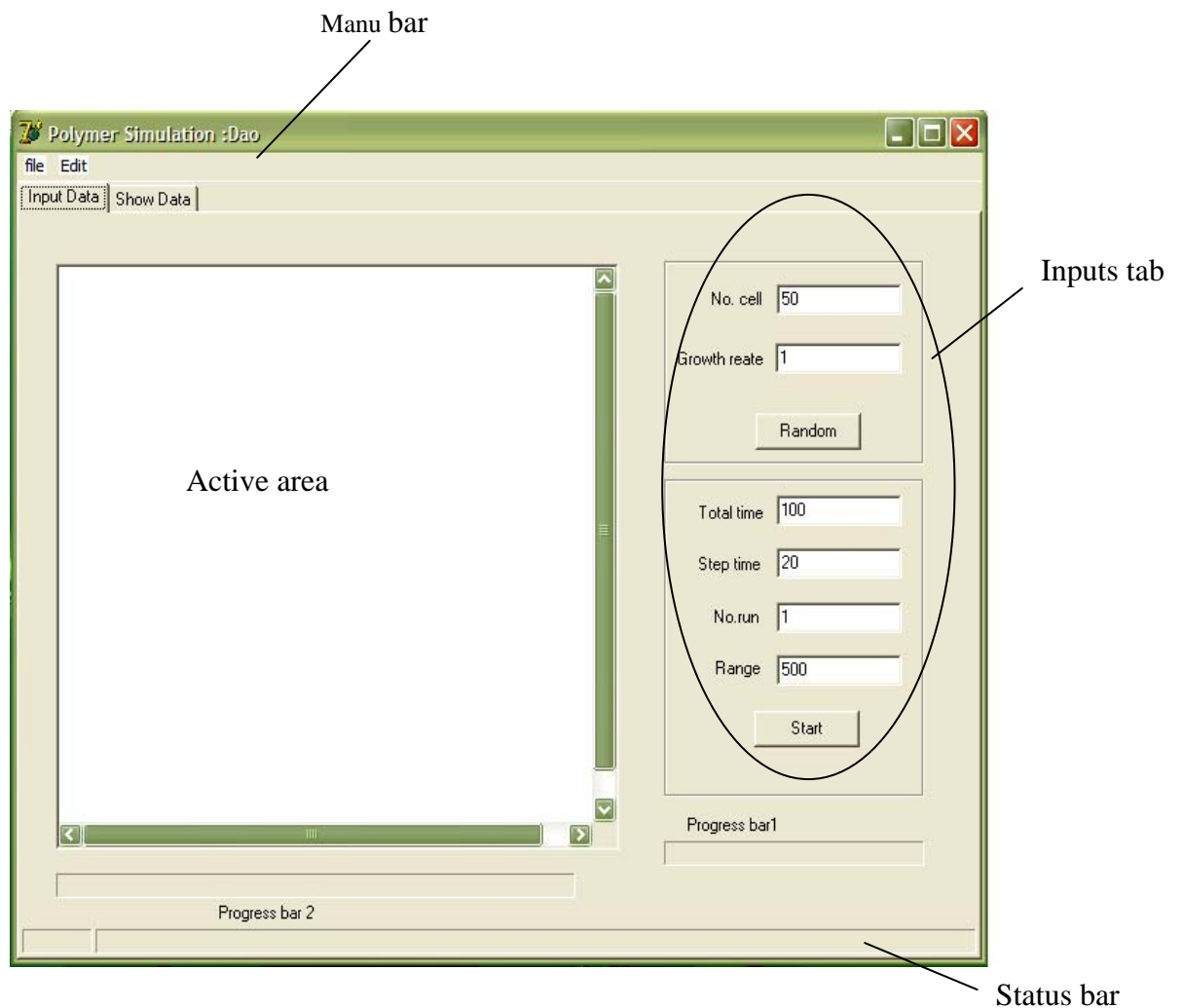
Polymer crystallization program were developed in this work to provide crystallization kinetics and detail morphological information at each crystallization time using the algorithm outline in Figure 2 and Figure 3. The code was developed by Borland Delphi. The program runs under Microsoft Windows XP on Personal PC. The program is simple to use and simulation results are given in both graphical form and spreadsheet (MS Excel file). The program is divided in to two parts for study effect of number of predetermined nuclei and growth rate (see Figure B1) and effect of crystallization temperature (see Figure B2). This appendix consists of both parts and provides step-by-step instructions for using the program

Polymer Crystallization Program for studying effect of number of predetermined nuclei and growth

When you start the Polymer Crystallization Program, the main window appears as Figure B1. All inputs are needed to be specified. At initial time, when click random button, the nuclei appear randomly in the active area and start growing when the start button is clicked. The information data at each time step are recorded until time reach to the total (final) time or complete crystallization. The text “Run Complete” and picture of crystals appears at the progress bar and active area respectively when finishes (see Figure B3). The parts of the main window are:

- Menu bar consist of 2 submenus that are file and edit. The file menu use for save data and picture obtained from simulation. The size of active area can be adjusted by edit menu.
- Input Data tab use for receive value of each parameters.
- Show Data tab use for show simulation results in text form (see Figure B2).
- Random button, numbers of predetermined nuclei appear randomly in the active area.

- Start button, the number of nuclei start growing by growth rate G until time equal to the total time.



Appendix Figure B1 The main window of Polymer Crystallization Program for study effect of number of predetermined nuclei and growth rate.

Polymer Simulation :Dao

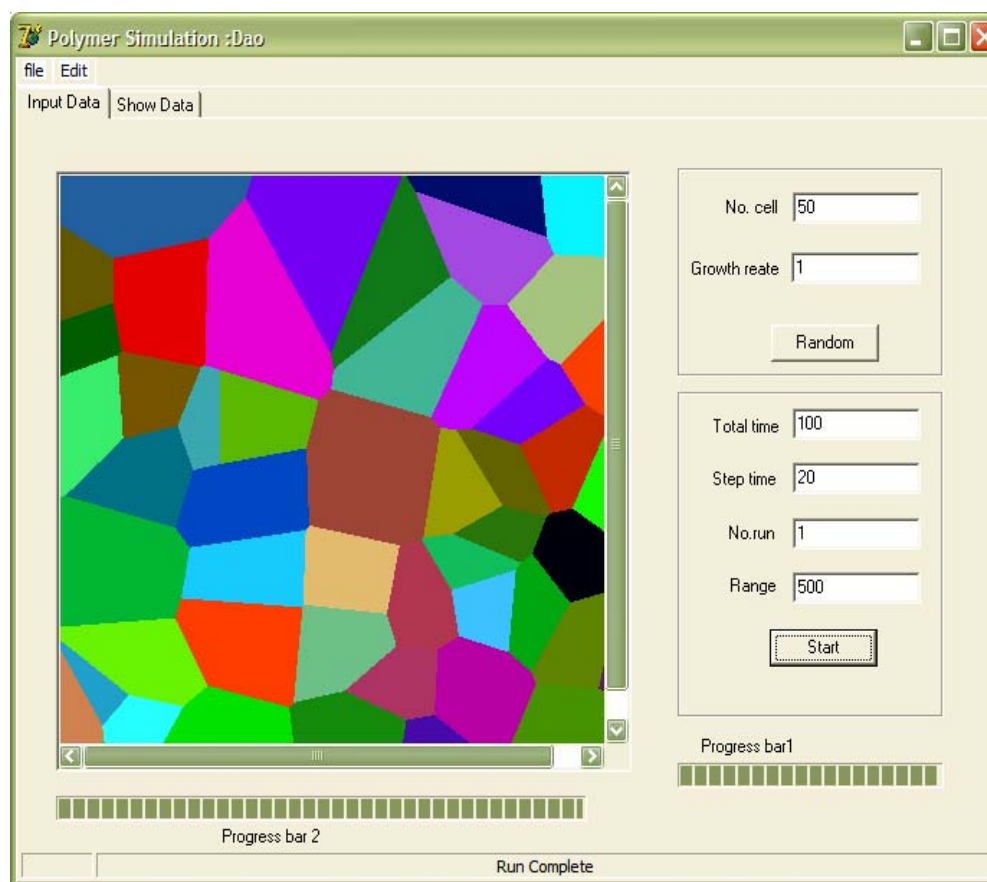
file Edit

Input Data Show Data

	t20	t40	t60	t80	t100	
13500-13999	0	0	0	0	0	
14000-14499	0	0	0	0	0	
14500-14999	0	0	0	0	0	
15000-15499	0	0	0	0	0	
15500-15999	0	0	0	0	0	
16000-16499	0	0	0	0	0	
16500-16999	0	0	0	0	0	
17000-17499	0	0	0	0	0	
area/total	30.02375	72.318125	92.1825	98.170625	99.5625	
area/No.cell	960.76	2314.18	2949.84	3141.46	3186	
Detail:						
No.cell	50					
No.cell	1					
Total time	100					
Step time	20					
No.run	1					
Range	500					

Show Table

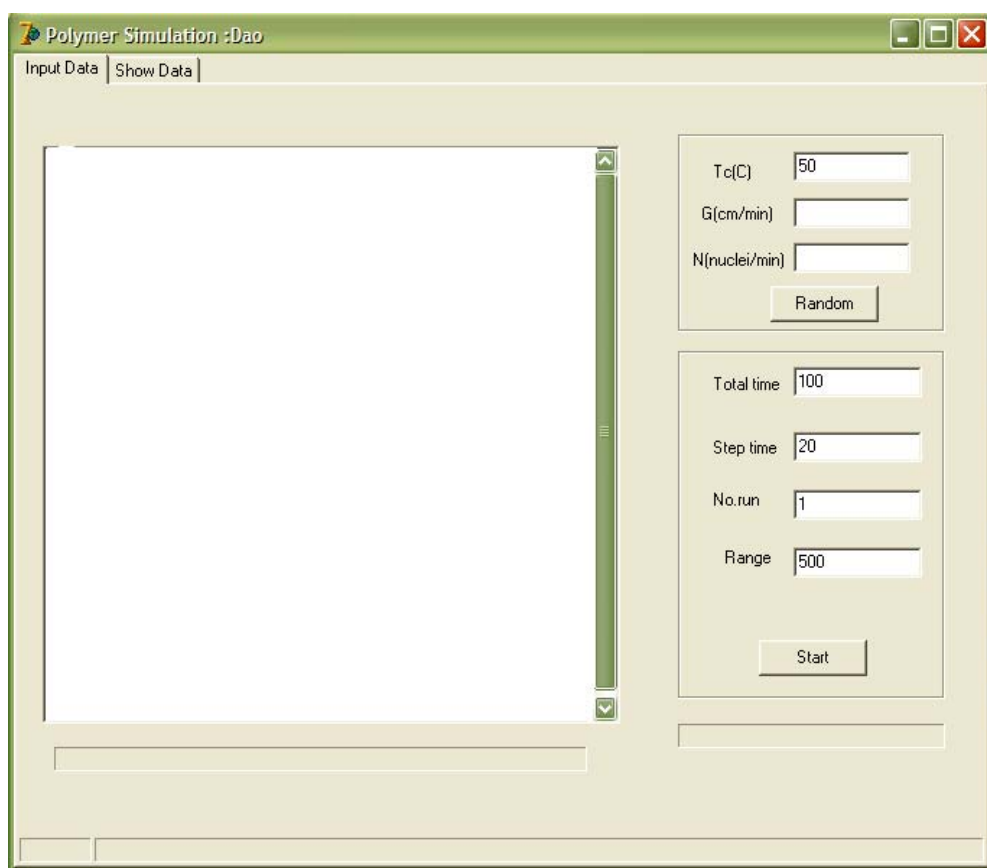
Appendix Figure B2 Outputs of the program in spreadsheet format.



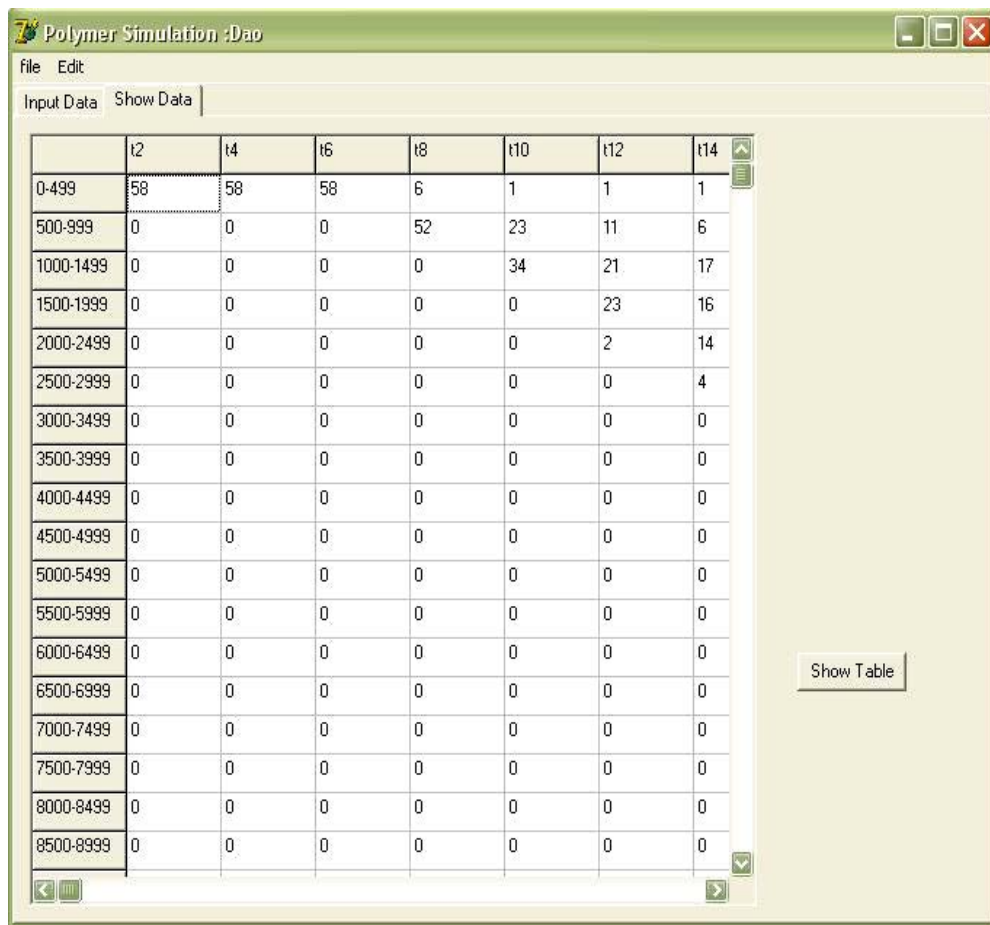
Appendix Figure B3 Outputs of the program in graphical format

Polymer Crystallization Program for studying effect crystallization temperature

The steps for using the program in this case are quite similar to previous case but only one crystallization parameter (i.e., crystallization temperature) is specified. The program use crystallization temperature to calculation of number of predetermined number of nuclei and growth rate. The Figure B4-B6 show the program windows.



Appendix Figure B4 The main window of Polymer Crystallization Program for study effect of crystallization temperature.



Polymer Simulation :Dao

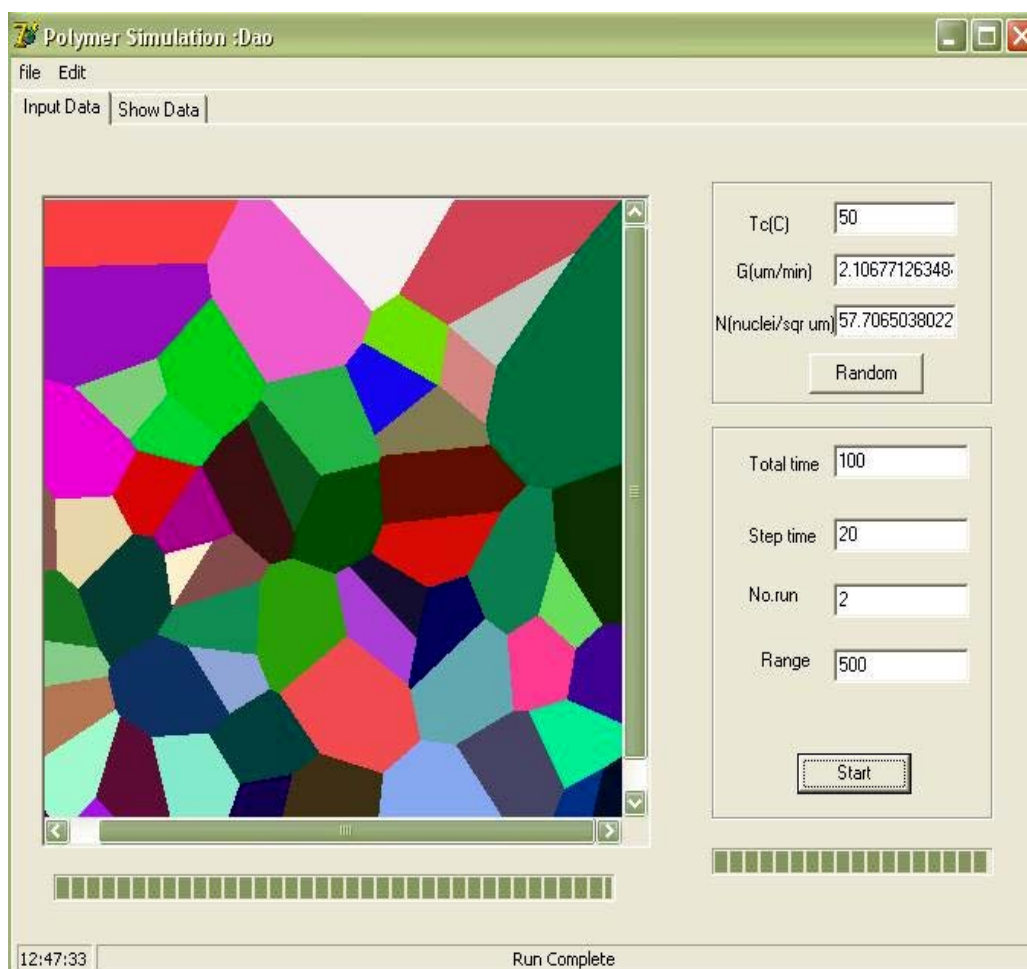
file Edit

Input Data Show Data

	t2	t4	t6	t8	t10	t12	t14
0-499	58	58	58	6	1	1	1
500-999	0	0	0	52	23	11	6
1000-1499	0	0	0	0	34	21	17
1500-1999	0	0	0	0	0	23	16
2000-2499	0	0	0	0	0	2	14
2500-2999	0	0	0	0	0	0	4
3000-3499	0	0	0	0	0	0	0
3500-3999	0	0	0	0	0	0	0
4000-4499	0	0	0	0	0	0	0
4500-4999	0	0	0	0	0	0	0
5000-5499	0	0	0	0	0	0	0
5500-5999	0	0	0	0	0	0	0
6000-6499	0	0	0	0	0	0	0
6500-6999	0	0	0	0	0	0	0
7000-7499	0	0	0	0	0	0	0
7500-7999	0	0	0	0	0	0	0
8000-8499	0	0	0	0	0	0	0
8500-8999	0	0	0	0	0	0	0

Show Table

Appendix Figure B5 Outputs of the program in spreadsheet format.



Appendix Figure B6 Outputs of the program in graphical format.