

ecNetSim

General-Purpose Electrochemical Simulation Software

(User Manual)

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I. Introduction

1.1 Purpose

This manual is written with the purpose to guide a user to carry out electrochemical simulations with the help of `ecNetSim`, a general-purpose electrochemical simulation package. It aims to help users become familiar with the software without external training. This manual provides detailed descriptions of the main features of `ecNetSim`, the input file format, and usage instructions.

1.2 Background

`ecNetSim` was developed by Dr. Zhao-Xiang Deng in the School of Chemistry and Materials Science, University of Science and Technology of China (USTC). The software has been used in Dr. Deng's course "Electroanalytical Chemistry" and his scientific research. Current users include the author himself, graduate students in his laboratory, students enrolled in related courses, as well as domestic and international scholars who have requested the software for their learning and research.

1.3 References

1. Zhao-Xiang Deng, Xiang-Qin Lin, Zhong-Hua Tong, Chinese J. Chem. 2004, 22, 719-726
2. Zhao-Xiang Deng, Zhong-Hua Tong, Xiang-Qin Lin, J. Electroanal. Chem. 2004, 568, 235-245
3. Zhao-Xiang Deng, Xiang-Qin Lin, Zhong-Hua Tong, Chinese J. Chem. 2005, 23, 166-172
4. Zhao-Xiang Deng, Xiang-Qin Lin, Zhong-Hua Tong, Chinese J. Chem. 2003, 21, 1137-1145
5. Zhao-Xiang Deng, Ph.D. Dissertation, USTC (Hefei, 2000)

II. Scope

2.1 Functions

As a program interface oriented toward the SPICE circuit simulation language, ecNetSim's primary function is to understand and compile arbitrary electrochemical/chemical reaction networks — that is, enabling the computer to read the reaction mechanisms, physicochemical parameters, and experimental conditions entered by the user, and convert them into SPICE circuit description language, so that appropriate circuit simulators can be invoked for computational solution.

This is achieved by defining a specific format and strictly following it to write a plain text file describing the electrochemical/chemical reaction mechanisms to be processed, along with given simulation parameters. This file is called the input file of the reaction compiler, named INPUT.ATN or any other user-defined name. ecNetSim correctly reads and understands this input file and automatically converts it into a SPICE circuit description file AUTONET.SP, which can then be directly used by a free circuit solver software such as LTspice (or a commercial software such as PSPICE) to execute user-defined simulations.

2.2 Performance

The software performs stably and meets most of user requirements.

2.3 Security

This software involves no security or confidentiality concerns. It is free for non-commercial use.

III. System Requirements

3.1 Hardware

The software runs on PCs. To ensure optimal performance, it is recommended that the computer has more than 2 GB RAM, more than 100 GB hard disk space, and at least an Intel Core i3 processor or higher.

3.2 Software

The software supports Windows operating systems. LTspice (free software) must be installed beforehand.

IV. Usage Instructions

4.1 Program Structure

The design flowchart of ecNetSim is shown in Figure 1. For ease of operation, this software does not use a graphical user interface; instead, it interacts with users through a plain-text input file (Figure 2). Users can conveniently define each input parameter and the operations to be performed within this text file. When the program runs, it automatically reads the input file and outputs the interpretation result (Figure 5), while calling corresponding subroutines to automatically generate SPICE circuit network description files (Figure 6). After ecNetSim successfully executes a user-defined input file (Figure 7), it displays a program interface shown in Figure 8, and invokes an external program LTspice (free software) upon user command to produce simulation results (Figure 9).

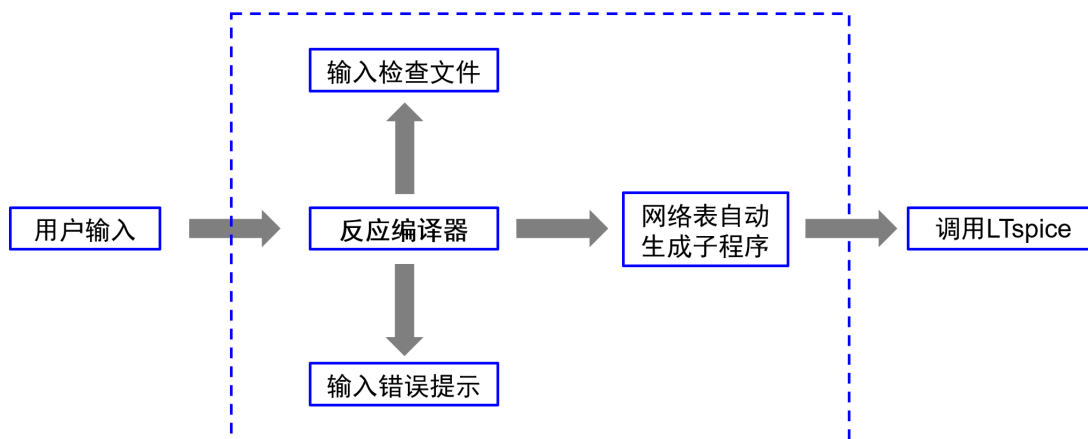


Figure 1. Design flowchart of the ecNetSim program

4.2 Input File

```
[Method(CV/CA: Cyclic Voltammetry/ChronoAmperometry)(no period)]
CV
[Number of Reaction-diffusion Species(no period)]
4
[Electron Transfer Reactions|E0(V)|arfa|na|k0(cm/s or s^-1 for SF)(with period)]
1+e<->2|0.0|0.5|1|1e-2;
3+e<->4|0.3|0.5|1|1e-2.
[Homogeneous Chemical Reactions|kfc|kbc(with period)]
2-->3|1e5|0;
1+4<->3+3|0.5|1e-2.
[Diffusion Type(L/S/C/RDE/FD/SF: Linear/Spherical/Cylindrical/Rotational
Disk/Finite Diffusion/SurFace)(no period)]
L
[Area(cm^2)/Radius(um)/Radius,Length(cm)/Angular Velocity(rad/s),Kinematic
Viscosity(cm^2/s),Area/Area,Thickness(cm)/Area(no period)]
0.0314
[Experimental: cycles,Ei(V),Es(V),Et(V),v(V/s) or Time(s) for CA,Temper(C.D.)(no
period)]
2,0.6,-0.4,0.6,1,25.0
[Simulation: boxnum,beta,dE(mV) or dt(s) for CA(no period)]
20,0.5,1
```

```

[IR drop: Ru(ohm),Cdl(F)(no period)]
0,0
[Initial Concentrations(mM or mol/cm^2 for SF)(with period)]
1|5;
2-4|0.
[Diffusion Coefficients(cm^2/s)(with period)]
1-4|5e-6.
[Current Output(CF/DF:Current Function/DeFault)(no period)]
DF
[Dimensionless Simulation Layer: Lmax(no period)]
6
[Do you want to run the simulation immediately(Y/N)?(no period)]
Y
[END]
*****
<A ECE-DISP SCHEME>

```

Figure 2. Format of the ecNetSim input file "INPUT.ATN"

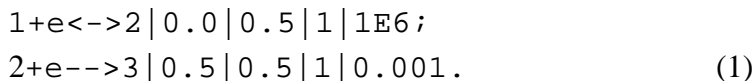
The ecNetSim input file is shown in Figure 2. Users should not modify the content within square brackets []. In the following, the different items in this file are explained in detail.

(1) Method Description: ecNetSim can simulate two types of transient experiments — cyclic voltammetry (CV) and chronoamperometry (CA), represented by the keywords CV (Cyclic Voltammetry) and CA (Chronoamperometry), respectively. If no entry is provided, cyclic voltammetry simulation is assumed by default.

(2) Number of Reaction-Diffusion Species: This is the total number of both electroactive and non-electroactive species that affect the system response.

(3) Electron Transfer Reactions: The reaction compiler uses a very convenient and intuitive method to describe electron transfer reactions and assign their thermodynamic and kinetic parameters. First, users must quote all electrochemical and chemical species with uniquely assigned numbers. The order of numbering is not important, but numbering must start from “1” and be consecutive. Species that have no effect on the overall system (e.g., products of certain irreversible reactions) may all be assigned number “0”.

For example, the following statement describes an "E_rE_i" process:



For heterogeneous reactions, the compiler recognizes the arrow "<->" as an electrochemically reversible or quasi-reversible reaction, while "-->" represents an electrochemically irreversible reaction. In these expressions, "+" indicates a reduction process, "-" indicates an oxidation process, "e" represents electrons (with optional

coefficient indicating the number of transferred electrons; defaults to 1 if omitted). Numbers 1, 2, 3 represent three species and simultaneously serve as their identifiers. Parameters separated by "|" after the reaction equation represent: formal (conditional) electrode potential E^0 , electron transfer coefficient α , n_a for multi-electron transfer processes, and standard heterogeneous rate constant k^0 . A statement containing the above information is called a reaction description line. Each line describes only one reaction; the last reaction description line ends with a period "." indicating all reaction descriptions are complete, while all other lines must end with ";". If species 3 does not undergo further reactions, its number can be changed to "0". *ecNetSim* can handle first-order single-electron or multi-electron heterogeneous transfer reactions.

(4) Homogeneous Chemical Reactions: The description of homogeneous chemical reactions is similar to that of heterogeneous reactions. Use "<->" for chemically reversible reactions and "-->" for chemically irreversible reactions. For irreversible reactions, in addition to this distinction, the reverse reaction rate constant must be set to zero. For example, the following expression describes two consecutive $C_{i2}C_r$ reactions:



The first reaction is an irreversible dimerization with a rate constant of $10^3 \text{ mM}^{-1} \text{ s}^{-1}$; the second is a first-order reversible reaction whose rate constants indicate it is a fast equilibrium process. *ecNetSim* requires every heterogeneous reaction to be first-order, and every chemical reaction to be an elementary step (in principle, elementary processes of any reaction order can be simulated). In principle, all non-elementary reactions can be "synthesized" using elementary processes. For example, the first-order reaction (for A) $2A \rightarrow C$ (slow) can be approximated by introducing two elementary reactions in the input file: $A \rightarrow B$ (slow); $B + A \rightarrow C$ (fast). Alternatively, this reaction can be directly described (for advanced users) upon modifying AUTONET.SP (the netlist file generated by *ecNetSim*). In fact, even more functions not mentioned in this manual can be realized by editing AUTONET.SP. Treatment of a purely homogeneous reaction system is also possible by simply setting method to CA, k^0 to 0, diffusion type to FD, boxnum to 1, and beta to 0.

(5) Diffusion Types: *ecNetSim* can simulate various forms of one-dimensional diffusion processes, including linear diffusion, spherical diffusion, cylindrical diffusion, rotating disk electrode (RDE), thin-layer finite diffusion, and surface processes (diffusionless). These are represented respectively by keywords L (Linear), S (Spherical), C (Cylindrical), RDE (Rotating Disk Electrode), FD (Finite Diffusion), and SF (SurFace). If left blank, linear diffusion is assumed by default.

(6) Electrode Parameters: Corresponding to each diffusion type, the user must enter specific electrode parameters to initiate a simulation. These include: planar electrode area (cm^2) for linear diffusion; spherical electrode radius (μm) for spherical diffusion; cylindrical electrode radius (μm)/length (cm) for cylindrical diffusion; angular velocity (rad/s)/kinematic viscosity (cm^2/s)/area (cm^2) for RDE.

(7) Experimental Parameters: Parameters related to electrochemical experiments include: number of scan cycles or potential steps (for chronoamperometry); initial potential E_i (V); switching potential E_s (V); terminating potential E_t (V); scan rate v (V/s) or total experimental time τ (s) (for chronoamperometry); temperature ($^\circ\text{C}$). Figures 3 and 4 illustrate potential sweep and potential step waveforms defined by these parameters, respectively.

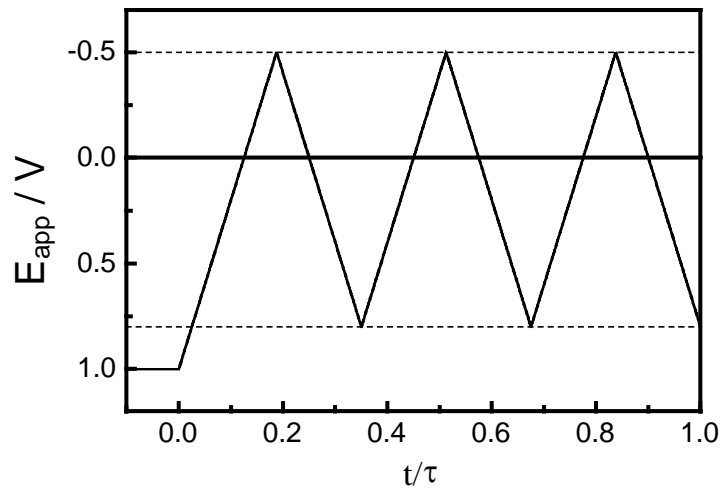


Figure 3. A potential waveform for cyclic voltammetry experiments. $E_i = 1.0 \text{ V}$, $E_s = -0.5 \text{ V}$, $E_t = 0.8 \text{ V}$, $v = 1.0 \text{ V s}^{-1}$, number of scan cycles is 3, total experimental time is τ

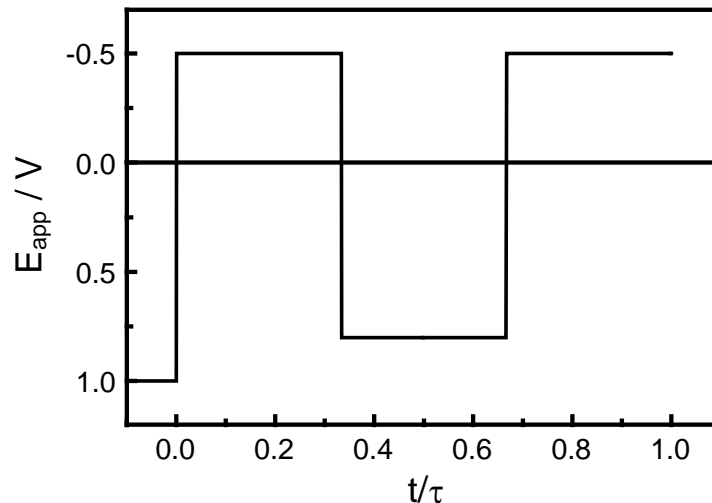


Figure 4. A potential waveform for potential step experiments. $E_i = 1.0$ V, $E_s = -0.5$ V, $E_t = 0.8$ V, number of potential steps is 3, total experimental time is τ

(8) Simulation Parameters: Here the user enters parameters required by the simulation algorithm itself, including: number of discretized spatial boxes, exponential grid expansion factor, and simulation potential increment (or time increment for chronoamperometry). Proper selection of simulation parameters directly affects numerical accuracy. Generally, more boxes and smaller potential/time increments yield more accurate results, but computation time increases accordingly; moderate values are generally recommended. Exponential grid expansion factor (β) relates to accuracy in complex ways: for linear diffusion, 0.5 is generally considered optimal, while other diffusion types differ. When coupled reactions exist, especially with reaction orders greater than 1, the situation becomes more complex. Preliminary trial calculations before formal simulation help determine suitable parameter values.

(9) Solution Resistance and Double-Layer Capacitance: `ecNetSim` can conveniently simulate voltammetric responses with iR drop. Users only need to provide values for uncompensated solution resistance R_u (Ω) and double-layer capacitance C_{dl} (F). When both are zero or omitted, ideal cell conditions (ohmic drop free, capacitive background free, infinitely fast cell/RC constant) are assumed.

(10) Initial Concentrations: Users enter initial concentrations for each species here. For bulk solution species, concentration unit is mM; for interfacial species, the surface concentration unit is mole/cm². Since a complicated system involves many species that mostly share the same initial concentrations, a concise input format is supported:

$$\begin{array}{l} 1, 2 | 0.1; \\ 3, 4-6 | 0. \end{array} \quad (3)$$

This means species 1 and 2 both have initial concentrations of 0.1 mM, while species 3, 4, 5, and 6 all have initial concentrations of 0.

(11) Diffusion Coefficients: Diffusion coefficient units are cm²/s. The input format is similar to concentrations. The following format specifies that species 1 through 5 all have diffusion coefficients of 10^{-5} cm²/s:

$$1-5 | 1E-5. \quad (4)$$

(12) Current Output Format: `ecNetSim` outputs two current forms simultaneously: dimensionless current and real current. Two options are available: DF and CF. The keyword CF indicates that all dimensionless currents are expressed as pseudo Current Functions (except for chronoamperometry and pure surface process simulations), as shown in equation 5:

$$\Psi_{\text{psd}} = \frac{i}{FAc_{\text{max}}^0 (F / RT)^{1/2} \nu^{1/2} D_{\text{max}}^{1/2}} \quad (5)$$

This format differs slightly from the Nicholson-Shain definition, mainly for easier handling of complex systems. Using the CF keyword forces `ecNetSim` to output pseudo current functions for all diffusion forms, making it easy to observe transitions from nonplanar/non-semi-infinite diffusion (e.g., spherical diffusion, thin-layer finite diffusion) toward linear semi-infinite diffusion under certain conditions, enabling an inter-system comparison.

Selecting DF or leaving it blank uses the system default values. For spherical electrodes, the dimensionless current is:

$$\Psi_{\text{S}} = \frac{i}{4\pi Fr_0 c_{\text{max}}^0 D_{\text{max}}} \quad (6)$$

where r_0 is the electrode radius, c_{max}^0 is the maximum initial concentration, D_{max} is the maximum diffusion coefficient, and F is Faraday's constant. For cylindrical electrodes:

$$\Psi_{\text{C}} = \frac{i}{2\pi Flc_{\text{max}}^0 D_{\text{max}}} \quad (7)$$

where l is the electrode length; other symbols are as above. For rotating disk electrodes:

$$\Psi_{\text{RDE}} = \frac{i}{0.620327 FAc_{\text{max}}^0 D_{\text{max}}^{2/3} \omega^{1/2} \nu^{-1/6}} \quad (8)$$

where A is the electrode area, ω is the angular velocity, ν is the kinematic viscosity; other symbols as above. For thin-layer finite diffusion:

$$\Psi_{\text{FD}} = \frac{4RTi}{F^2 Alc_{\text{max}}^0 \nu} \quad (9)$$

where l is the thin-layer cell thickness, ν is the scan rate, R is the gas constant; other symbols as above. For surface processes:

$$\Psi_{\text{SF}} = \frac{4RTi}{F^2 A\Gamma_{\text{max}}^0 \nu} \quad (10)$$

where Γ_{\max}^0 is the maximum initial surface concentration (surface excess); other symbols as above. In chronoamperometry simulations, finite diffusion and surface process only produce real currents. For linear diffusion in CA mode, the default dimensionless current is defined so that its value equals 1 when $t = \tau$ for a Cottrell process:

$$\Psi_L = \frac{i}{FAc_{\max}^0 (\pi\tau)^{-1/2} D_{\max}^{1/2}} \quad (11)$$

(13) Dimensionless Simulation Layer Thickness: Default is 6 for semi-infinite linear, spherical, or cylindrical diffusion, meaning the semi-infinite boundary is at $6(D_{\max}\tau)^{1/2}$. Users may change the default here. For RDE processes, the default is 3, meaning the right boundary of the simulation layer is at $3\delta_{\max}$ (where δ_{\max} is the steady-state diffusion layer thickness for the species with the largest diffusion coefficient). Users can modify this default. For RDE, entering "2.5delta_max" forces the simulation layer thickness to $2.5\delta_{\max}$; entering "2.5" (without the appending delta_max switch) means the layer thickness is $2.5(D_{\max}\tau)^{1/2}$.

(14) Run Simulation Immediately? Answer Y to execute the simulation immediately after generating the network model; N to generate the model without immediate execution (AUTONET.SP can be loaded manually for later simulation).

(15) End-of-File Marker: The end marker recognized by the compiler is [END]. When the compiler reads this point, it stops reading further; all content after this marker is ignored. Therefore, users may freely add comments after [END].

4.3 Output Files

ecNetSim first scans the input file line by line, stores relevant parameters, and automatically identifies each electrochemical/chemical reaction expression, storing reaction information including reaction structure and thermodynamic/kinetic parameters according to a defined scheme. It then generates two files: INPUT.ATN.CHK (Figure 5) and AUTONET.SP (Figure 6). The former is ecNetSim's interpretation of the input file, used for error checking; the latter is the SPICE-based circuit description file, which can be read and executed by LTspice for simulation. Advanced users can simulate additional electrochemical/chemical problems by directly modifying the AUTONET.SP file, providing convenience for developing new simulation capabilities. These extra functions have been implemented in the "Electroanalytical Chemistry" course taught by the software author at USTC for graduate students, including electrochemical impedance spectroscopy, AC voltammetry, differential pulse voltammetry, square wave voltammetry, staircase voltammetry, and chemical oscillation reactions.

```
[Method(CV/CA: Cyclic Voltammetry/ChronoAmperometry)(no period)]
cyclic voltammetry
[Number of Reaction-diffusion Species(no period)]
4
[Electron Transfer Reactions|E0(V)|arfa|na|k0(cm/s or s^-1 for SF)(with period)]
Ox: 1 | n: 1 | Red: 2 | E0: 0 | arfa: .5 | arfa2: .5 | na: 1 | k0: .01
Ox: 3 | n: 1 | Red: 4 | E0: .3 | arfa: .5 | arfa2: .5 | na: 1 | k0: .01
[Homogeneous Chemical Reactions|kfc|kbc(with period)]
reactant: 2| product: 3| kfc: 100000 | kbc: 0
reactant: 1 4| product: 3 3| kfc: .5 | kbc: .01
[Diffusion Type(L/S/C/RDE/FD/SF: Linear/Spherical/Cylindrical/Rotational
Disk/Finite Diffusion/SurFace)(no period)]
linear
[Area(cm^2)/Radius(um)/Radius,Length(cm)/Angular Velocity(rad/s),Kinematic
Viscosity(cm^2/s),Area/Area,Thickness(cm)/Area(no period)]
area= .0314
[Experimental: cycles,Ei(V),Es(V),Et(V),v(V/s) or Time(s) for CA,Temper(C.D.)(no
period)]
cycles= 2 | Ei= .6 | Es=-.4 | Et= .6 | v= 1 | Temper= 25
[Simulation: boxnum,beta,dE(mV) or dt(s) for CA(no period)]
boxnum= 20 | beta= .5 | dE= 1
[IR drop: Ru(ohm),Cdl(F)(no period)]
Ru= 0 | Cdl= 0
[Initial Concentrations(mM or mol/cm^2 for SF)(with period)]
1 5
2 0
3 0
4 0
[Diffusion Coefficients(cm^2/s)(with period)]
1 .000005
2 .000005
3 .000005
4 .000005
[Current Output(CF/DF:Current Function/DeFault)(no period)]
default
[Dimensionless Simulation Layer: Lmax(no period)]
Lmax= 6
[Do you want to run the simulation immediately(Y/N)?(no period)]
Yes
[END]
```

Figure 5. Format of the input-checking file "INPUT.ATN.CHK"

C:\software\NETSIM64\LTSPICE\AUTONET.SP Created by ecNETSIM.

C_Cslz1 slz1 0 1.767194E-04 IC=1
R_Rslz1 slz1 slz2 2.269122E-04
C_Cslz2 slz2 0 2.913611E-04 IC=1
R_Rslz2 slz2 slz3 3.74115E-04
C_Cslz3 slz3 0 4.803732E-04 IC=1
R_Rslz3 slz3 slz4 6.168114E-04
C_Cslz4 slz4 0 7.920015E-04 IC=1
R_Rslz4 slz4 slz5 1.01695E-03
C_Cslz5 slz5 0 1.30579E-03 IC=1
R_Rslz5 slz5 slz6 1.676667E-03
C_Cslz6 slz6 0 2.152883E-03 IC=1
R_Rslz6 slz6 slz7 2.764357E-03
C_Cslz7 slz7 0 3.549504E-03 IC=1
R_Rslz7 slz7 slz8 4.557654E-03
C_Cslz8 slz8 0 5.852143E-03 IC=1
R_Rslz8 slz8 slz9 7.514302E-03
C_Cslz9 slz9 0 9.648553E-03 IC=1
R_Rslz9 slz9 slz10 1.238899E-02
C_Cslz10 slz10 0 1.590778E-02 IC=1
R_Rslz10 slz10 slz11 2.042599E-02
C_Cslz11 slz11 0 2.622749E-02 IC=1
R_Rslz11 slz11 slz12 3.367676E-02
C_Cslz12 slz12 0 4.324182E-02 IC=1
R_Rslz12 slz12 slz13 .0555236
C_Cslz13 slz13 0 .0712937 IC=1
R_Rslz13 slz13 slz14 9.154291E-02
C_Cslz14 slz14 0 .1175434 IC=1
R_Rslz14 slz14 slz15 .1509288
C_Cslz15 slz15 0 .1937964 IC=1
R_Rslz15 slz15 slz16 .2488394
C_Cslz16 slz16 0 .3195162 IC=1
R_Rslz16 slz16 slz17 .410267
C_Cslz17 slz17 0 .5267932 IC=1
R_Rslz17 slz17 slz18 .6764158
C_Cslz18 slz18 0 .8685351 IC=1
R_Rslz18 slz18 slz19 1.115221
C_Cslz19 slz19 0 1.431972 IC=1
R_Rslz19 slz19 slz20 1.838689
C_Cslz20 slz20 0 2.360923 IC=1
R_Rslz20 slz20 slz21 3.031486

*Network Model for No.1 species Ends Here

C_Cs2z1 s2z1 0 1.767194E-04 IC=0
R_Rs2z1 s2z1 s2z2 2.269122E-04
C_Cs2z2 s2z2 0 2.913611E-04 IC=0
R_Rs2z2 s2z2 s2z3 3.74115E-04
C_Cs2z3 s2z3 0 4.803732E-04 IC=0
R_Rs2z3 s2z3 s2z4 6.168114E-04
C_Cs2z4 s2z4 0 7.920015E-04 IC=0
R_Rs2z4 s2z4 s2z5 1.01695E-03
C_Cs2z5 s2z5 0 1.30579E-03 IC=0
R_Rs2z5 s2z5 s2z6 1.676667E-03
C_Cs2z6 s2z6 0 2.152883E-03 IC=0
R_Rs2z6 s2z6 s2z7 2.764357E-03
C_Cs2z7 s2z7 0 3.549504E-03 IC=0
R_Rs2z7 s2z7 s2z8 4.557654E-03
C_Cs2z8 s2z8 0 5.852143E-03 IC=0
R_Rs2z8 s2z8 s2z9 7.514302E-03
C_Cs2z9 s2z9 0 9.648553E-03 IC=0
R_Rs2z9 s2z9 s2z10 1.238899E-02
C_Cs2z10 s2z10 0 1.590778E-02 IC=0
R_Rs2z10 s2z10 s2z11 2.042599E-02
C_Cs2z11 s2z11 0 2.622749E-02 IC=0
R_Rs2z11 s2z11 s2z12 3.367676E-02
C_Cs2z12 s2z12 0 4.324182E-02 IC=0
R_Rs2z12 s2z12 s2z13 .0555236
C_Cs2z13 s2z13 0 .0712937 IC=0
R_Rs2z13 s2z13 s2z14 9.154291E-02

C_Cs2z14	s2z14	0	.1175434	IC=0
R_Rs2z14	s2z14	s2z15	.1509288	
C_Cs2z15	s2z15	0	.1937964	IC=0
R_Rs2z15	s2z15	s2z16	.2488394	
C_Cs2z16	s2z16	0	.3195162	IC=0
R_Rs2z16	s2z16	s2z17	.410267	
C_Cs2z17	s2z17	0	.5267932	IC=0
R_Rs2z17	s2z17	s2z18	.6764158	
C_Cs2z18	s2z18	0	.8685351	IC=0
R_Rs2z18	s2z18	s2z19	1.115221	
C_Cs2z19	s2z19	0	1.431972	IC=0
R_Rs2z19	s2z19	s2z20	1.838689	
C_Cs2z20	s2z20	0	2.360923	IC=0
R_Rs2z20	s2z20	s2z21	3.031486	

*Network Model for No.2 species Ends Here

C_Cs3z1	s3z1	0	1.767194E-04	IC=0
R_Rs3z1	s3z1	s3z2	2.269122E-04	
C_Cs3z2	s3z2	0	2.913611E-04	IC=0
R_Rs3z2	s3z2	s3z3	3.74115E-04	
C_Cs3z3	s3z3	0	4.803732E-04	IC=0
R_Rs3z3	s3z3	s3z4	6.168114E-04	
C_Cs3z4	s3z4	0	7.920015E-04	IC=0
R_Rs3z4	s3z4	s3z5	1.01695E-03	
C_Cs3z5	s3z5	0	1.30579E-03	IC=0
R_Rs3z5	s3z5	s3z6	1.676667E-03	
C_Cs3z6	s3z6	0	2.152883E-03	IC=0
R_Rs3z6	s3z6	s3z7	2.764357E-03	
C_Cs3z7	s3z7	0	3.549504E-03	IC=0
R_Rs3z7	s3z7	s3z8	4.557654E-03	
C_Cs3z8	s3z8	0	5.852143E-03	IC=0
R_Rs3z8	s3z8	s3z9	7.514302E-03	
C_Cs3z9	s3z9	0	9.648553E-03	IC=0
R_Rs3z9	s3z9	s3z10	1.238899E-02	
C_Cs3z10	s3z10	0	1.590778E-02	IC=0
R_Rs3z10	s3z10	s3z11	2.042599E-02	
C_Cs3z11	s3z11	0	2.622749E-02	IC=0
R_Rs3z11	s3z11	s3z12	3.367676E-02	
C_Cs3z12	s3z12	0	4.324182E-02	IC=0
R_Rs3z12	s3z12	s3z13	.0555236	
C_Cs3z13	s3z13	0	.0712937	IC=0
R_Rs3z13	s3z13	s3z14	9.154291E-02	
C_Cs3z14	s3z14	0	.1175434	IC=0
R_Rs3z14	s3z14	s3z15	.1509288	
C_Cs3z15	s3z15	0	.1937964	IC=0
R_Rs3z15	s3z15	s3z16	.2488394	
C_Cs3z16	s3z16	0	.3195162	IC=0
R_Rs3z16	s3z16	s3z17	.410267	
C_Cs3z17	s3z17	0	.5267932	IC=0
R_Rs3z17	s3z17	s3z18	.6764158	
C_Cs3z18	s3z18	0	.8685351	IC=0
R_Rs3z18	s3z18	s3z19	1.115221	
C_Cs3z19	s3z19	0	1.431972	IC=0
R_Rs3z19	s3z19	s3z20	1.838689	
C_Cs3z20	s3z20	0	2.360923	IC=0
R_Rs3z20	s3z20	s3z21	3.031486	

*Network Model for No.3 species Ends Here

C_Cs4z1	s4z1	0	1.767194E-04	IC=0
R_Rs4z1	s4z1	s4z2	2.269122E-04	
C_Cs4z2	s4z2	0	2.913611E-04	IC=0
R_Rs4z2	s4z2	s4z3	3.74115E-04	
C_Cs4z3	s4z3	0	4.803732E-04	IC=0
R_Rs4z3	s4z3	s4z4	6.168114E-04	
C_Cs4z4	s4z4	0	7.920015E-04	IC=0
R_Rs4z4	s4z4	s4z5	1.01695E-03	
C_Cs4z5	s4z5	0	1.30579E-03	IC=0
R_Rs4z5	s4z5	s4z6	1.676667E-03	
C_Cs4z6	s4z6	0	2.152883E-03	IC=0

R_Rs4z6	s4z6 s4z7	2.764357E-03
C_Cs4z7	s4z7 0	3.549504E-03 IC=0
R_Rs4z7	s4z7 s4z8	4.557654E-03
C_Cs4z8	s4z8 0	5.852143E-03 IC=0
R_Rs4z8	s4z8 s4z9	7.514302E-03
C_Cs4z9	s4z9 0	9.648553E-03 IC=0
R_Rs4z9	s4z9 s4z10	1.238899E-02
C_Cs4z10	s4z10 0	1.590778E-02 IC=0
R_Rs4z10	s4z10 s4z11	2.042599E-02
C_Cs4z11	s4z11 0	2.622749E-02 IC=0
R_Rs4z11	s4z11 s4z12	3.367676E-02
C_Cs4z12	s4z12 0	4.324182E-02 IC=0
R_Rs4z12	s4z12 s4z13	.0555236
C_Cs4z13	s4z13 0	.0712937 IC=0
R_Rs4z13	s4z13 s4z14	9.154291E-02
C_Cs4z14	s4z14 0	.1175434 IC=0
R_Rs4z14	s4z14 s4z15	.1509288
C_Cs4z15	s4z15 0	.1937964 IC=0
R_Rs4z15	s4z15 s4z16	.2488394
C_Cs4z16	s4z16 0	.3195162 IC=0
R_Rs4z16	s4z16 s4z17	.410267
C_Cs4z17	s4z17 0	.5267932 IC=0
R_Rs4z17	s4z17 s4z18	.6764158
C_Cs4z18	s4z18 0	.8685351 IC=0
R_Rs4z18	s4z18 s4z19	1.115221
C_Cs4z19	s4z19 0	1.431972 IC=0
R_Rs4z19	s4z19 s4z20	1.838689
C_Cs4z20	s4z20 0	2.360923 IC=0
R_Rs4z20	s4z20 s4z21	3.031486

*Network Model for No.4 species Ends Here

G_Gs2z1r1	s2z1 0	VALUE = { 400000*V(s2z1)*1.767194E-04 }
G_Gs2z2r1	s2z2 0	VALUE = { 400000*V(s2z2)*2.913611E-04 }
G_Gs2z3r1	s2z3 0	VALUE = { 400000*V(s2z3)*4.803732E-04 }
G_Gs2z4r1	s2z4 0	VALUE = { 400000*V(s2z4)*7.920015E-04 }
G_Gs2z5r1	s2z5 0	VALUE = { 400000*V(s2z5)*1.30579E-03 }
G_Gs2z6r1	s2z6 0	VALUE = { 400000*V(s2z6)*2.152883E-03 }
G_Gs2z7r1	s2z7 0	VALUE = { 400000*V(s2z7)*3.549504E-03 }
G_Gs2z8r1	s2z8 0	VALUE = { 400000*V(s2z8)*5.852143E-03 }
G_Gs2z9r1	s2z9 0	VALUE = { 400000*V(s2z9)*9.648553E-03 }
G_Gs2z10r1	s2z10 0	VALUE = { 400000*V(s2z10)*1.590778E-02 }
G_Gs2z11r1	s2z11 0	VALUE = { 400000*V(s2z11)*2.622749E-02 }
G_Gs2z12r1	s2z12 0	VALUE = { 400000*V(s2z12)*4.324182E-02 }
G_Gs2z13r1	s2z13 0	VALUE = { 400000*V(s2z13)*.0712937 }
G_Gs2z14r1	s2z14 0	VALUE = { 400000*V(s2z14)*.1175434 }
G_Gs2z15r1	s2z15 0	VALUE = { 400000*V(s2z15)*.1937964 }
G_Gs2z16r1	s2z16 0	VALUE = { 400000*V(s2z16)*.3195162 }
G_Gs2z17r1	s2z17 0	VALUE = { 400000*V(s2z17)*.5267932 }
G_Gs2z18r1	s2z18 0	VALUE = { 400000*V(s2z18)*.8685351 }
G_Gs2z19r1	s2z19 0	VALUE = { 400000*V(s2z19)*1.431972 }
G_Gs2z20r1	s2z20 0	VALUE = { 400000*V(s2z20)*2.360923 }

*Homogeneous Kinetics Item for No.2 species as An Reactant at the No.1 Chemical Reaction Ends Here

G_Gs3z1r2	s3z1 0	VALUE = { -400000*V(s2z1)*1.767194E-04 }
G_Gs3z2r2	s3z2 0	VALUE = { -400000*V(s2z2)*2.913611E-04 }
G_Gs3z3r2	s3z3 0	VALUE = { -400000*V(s2z3)*4.803732E-04 }
G_Gs3z4r2	s3z4 0	VALUE = { -400000*V(s2z4)*7.920015E-04 }
G_Gs3z5r2	s3z5 0	VALUE = { -400000*V(s2z5)*1.30579E-03 }
G_Gs3z6r2	s3z6 0	VALUE = { -400000*V(s2z6)*2.152883E-03 }
G_Gs3z7r2	s3z7 0	VALUE = { -400000*V(s2z7)*3.549504E-03 }
G_Gs3z8r2	s3z8 0	VALUE = { -400000*V(s2z8)*5.852143E-03 }
G_Gs3z9r2	s3z9 0	VALUE = { -400000*V(s2z9)*9.648553E-03 }
G_Gs3z10r2	s3z10 0	VALUE = { -400000*V(s2z10)*1.590778E-02 }
G_Gs3z11r2	s3z11 0	VALUE = { -400000*V(s2z11)*2.622749E-02 }
G_Gs3z12r2	s3z12 0	VALUE = { -400000*V(s2z12)*4.324182E-02 }
G_Gs3z13r2	s3z13 0	VALUE = { -400000*V(s2z13)*.0712937 }
G_Gs3z14r2	s3z14 0	VALUE = { -400000*V(s2z14)*.1175434 }
G_Gs3z15r2	s3z15 0	VALUE = { -400000*V(s2z15)*.1937964 }

G_Gs3z16r2	s3z16	0	VALUE =	{ -400000*V(s2z16)*.3195162 }
G_Gs3z17r2	s3z17	0	VALUE =	{ -400000*V(s2z17)*.5267932 }
G_Gs3z18r2	s3z18	0	VALUE =	{ -400000*V(s2z18)*.8685351 }
G_Gs3z19r2	s3z19	0	VALUE =	{ -400000*V(s2z19)*1.431972 }
G_Gs3z20r2	s3z20	0	VALUE =	{ -400000*V(s2z20)*2.360923 }

*Homogeneous Kinetics Item for No.3 species as An Product at the No.1 Chemical Reaction Ends Here

G_Gslz1r3	slz1	0	VALUE =	{ 10*V(slz1)*V(s4z1)*1.767194E-04 }
G_Gslz2r3	slz2	0	VALUE =	{ 10*V(slz2)*V(s4z2)*2.913611E-04 }
G_Gslz3r3	slz3	0	VALUE =	{ 10*V(slz3)*V(s4z3)*4.803732E-04 }
G_Gslz4r3	slz4	0	VALUE =	{ 10*V(slz4)*V(s4z4)*7.920015E-04 }
G_Gslz5r3	slz5	0	VALUE =	{ 10*V(slz5)*V(s4z5)*1.30579E-03 }
G_Gslz6r3	slz6	0	VALUE =	{ 10*V(slz6)*V(s4z6)*2.152883E-03 }
G_Gslz7r3	slz7	0	VALUE =	{ 10*V(slz7)*V(s4z7)*3.549504E-03 }
G_Gslz8r3	slz8	0	VALUE =	{ 10*V(slz8)*V(s4z8)*5.852143E-03 }
G_Gslz9r3	slz9	0	VALUE =	{ 10*V(slz9)*V(s4z9)*9.648553E-03 }
G_Gslz10r3	slz10	0	VALUE =	{ 10*V(slz10)*V(s4z10)*1.590778E-02 }
G_Gslz11r3	slz11	0	VALUE =	{ 10*V(slz11)*V(s4z11)*2.622749E-02 }
G_Gslz12r3	slz12	0	VALUE =	{ 10*V(slz12)*V(s4z12)*4.324182E-02 }
G_Gslz13r3	slz13	0	VALUE =	{ 10*V(slz13)*V(s4z13)*.0712937 }
G_Gslz14r3	slz14	0	VALUE =	{ 10*V(slz14)*V(s4z14)*.1175434 }
G_Gslz15r3	slz15	0	VALUE =	{ 10*V(slz15)*V(s4z15)*.1937964 }
G_Gslz16r3	slz16	0	VALUE =	{ 10*V(slz16)*V(s4z16)*.3195162 }
G_Gslz17r3	slz17	0	VALUE =	{ 10*V(slz17)*V(s4z17)*.5267932 }
G_Gslz18r3	slz18	0	VALUE =	{ 10*V(slz18)*V(s4z18)*.8685351 }
G_Gslz19r3	slz19	0	VALUE =	{ 10*V(slz19)*V(s4z19)*1.431972 }
G_Gslz20r3	slz20	0	VALUE =	{ 10*V(slz20)*V(s4z20)*2.360923 }

*Homogeneous Kinetics Item for No.1 species as An Reactant at the No.2 Chemical Reaction Ends Here

G_Gs4z1r4	s4z1	0	VALUE =	{ 10*V(slz1)*V(s4z1)*1.767194E-04 }
G_Gs4z2r4	s4z2	0	VALUE =	{ 10*V(slz2)*V(s4z2)*2.913611E-04 }
G_Gs4z3r4	s4z3	0	VALUE =	{ 10*V(slz3)*V(s4z3)*4.803732E-04 }
G_Gs4z4r4	s4z4	0	VALUE =	{ 10*V(slz4)*V(s4z4)*7.920015E-04 }
G_Gs4z5r4	s4z5	0	VALUE =	{ 10*V(slz5)*V(s4z5)*1.30579E-03 }
G_Gs4z6r4	s4z6	0	VALUE =	{ 10*V(slz6)*V(s4z6)*2.152883E-03 }
G_Gs4z7r4	s4z7	0	VALUE =	{ 10*V(slz7)*V(s4z7)*3.549504E-03 }
G_Gs4z8r4	s4z8	0	VALUE =	{ 10*V(slz8)*V(s4z8)*5.852143E-03 }
G_Gs4z9r4	s4z9	0	VALUE =	{ 10*V(slz9)*V(s4z9)*9.648553E-03 }
G_Gs4z10r4	s4z10	0	VALUE =	{ 10*V(slz10)*V(s4z10)*1.590778E-02 }
G_Gs4z11r4	s4z11	0	VALUE =	{ 10*V(slz11)*V(s4z11)*2.622749E-02 }
G_Gs4z12r4	s4z12	0	VALUE =	{ 10*V(slz12)*V(s4z12)*4.324182E-02 }
G_Gs4z13r4	s4z13	0	VALUE =	{ 10*V(slz13)*V(s4z13)*.0712937 }
G_Gs4z14r4	s4z14	0	VALUE =	{ 10*V(slz14)*V(s4z14)*.1175434 }
G_Gs4z15r4	s4z15	0	VALUE =	{ 10*V(slz15)*V(s4z15)*.1937964 }
G_Gs4z16r4	s4z16	0	VALUE =	{ 10*V(slz16)*V(s4z16)*.3195162 }
G_Gs4z17r4	s4z17	0	VALUE =	{ 10*V(slz17)*V(s4z17)*.5267932 }
G_Gs4z18r4	s4z18	0	VALUE =	{ 10*V(slz18)*V(s4z18)*.8685351 }
G_Gs4z19r4	s4z19	0	VALUE =	{ 10*V(slz19)*V(s4z19)*1.431972 }
G_Gs4z20r4	s4z20	0	VALUE =	{ 10*V(slz20)*V(s4z20)*2.360923 }

*Homogeneous Kinetics Item for No.4 species as An Reactant at the No.2 Chemical Reaction Ends Here

G_Gs3z1r5	s3z1	0	VALUE =	{ -10*V(slz1)*V(s4z1)*1.767194E-04 }
G_Gs3z2r5	s3z2	0	VALUE =	{ -10*V(slz2)*V(s4z2)*2.913611E-04 }
G_Gs3z3r5	s3z3	0	VALUE =	{ -10*V(slz3)*V(s4z3)*4.803732E-04 }
G_Gs3z4r5	s3z4	0	VALUE =	{ -10*V(slz4)*V(s4z4)*7.920015E-04 }
G_Gs3z5r5	s3z5	0	VALUE =	{ -10*V(slz5)*V(s4z5)*1.30579E-03 }
G_Gs3z6r5	s3z6	0	VALUE =	{ -10*V(slz6)*V(s4z6)*2.152883E-03 }
G_Gs3z7r5	s3z7	0	VALUE =	{ -10*V(slz7)*V(s4z7)*3.549504E-03 }
G_Gs3z8r5	s3z8	0	VALUE =	{ -10*V(slz8)*V(s4z8)*5.852143E-03 }
G_Gs3z9r5	s3z9	0	VALUE =	{ -10*V(slz9)*V(s4z9)*9.648553E-03 }
G_Gs3z10r5	s3z10	0	VALUE =	{ -10*V(slz10)*V(s4z10)*1.590778E-02 }
G_Gs3z11r5	s3z11	0	VALUE =	{ -10*V(slz11)*V(s4z11)*2.622749E-02 }
G_Gs3z12r5	s3z12	0	VALUE =	{ -10*V(slz12)*V(s4z12)*4.324182E-02 }
G_Gs3z13r5	s3z13	0	VALUE =	{ -10*V(slz13)*V(s4z13)*.0712937 }
G_Gs3z14r5	s3z14	0	VALUE =	{ -10*V(slz14)*V(s4z14)*.1175434 }

G_Gs3z15r5	s3z15	0	VALUE =	{	-10*v(s1z15)*v(s4z15)*.1937964	}
G_Gs3z16r5	s3z16	0	VALUE =	{	-10*v(s1z16)*v(s4z16)*.3195162	}
G_Gs3z17r5	s3z17	0	VALUE =	{	-10*v(s1z17)*v(s4z17)*.5267932	}
G_Gs3z18r5	s3z18	0	VALUE =	{	-10*v(s1z18)*v(s4z18)*.8685351	}
G_Gs3z19r5	s3z19	0	VALUE =	{	-10*v(s1z19)*v(s4z19)*1.431972	}
G_Gs3z20r5	s3z20	0	VALUE =	{	-10*v(s1z20)*v(s4z20)*2.360923	}

*Homogeneous Kinetics Item for No.3 species as An Product at the No.2 Chemical Reaction Ends Here

G_Gs3z1r6	s3z1	0	VALUE =	{	-10*v(s1z1)*v(s4z1)*1.767194E-04	}
G_Gs3z2r6	s3z2	0	VALUE =	{	-10*v(s1z2)*v(s4z2)*2.913611E-04	}
G_Gs3z3r6	s3z3	0	VALUE =	{	-10*v(s1z3)*v(s4z3)*4.803732E-04	}
G_Gs3z4r6	s3z4	0	VALUE =	{	-10*v(s1z4)*v(s4z4)*7.920015E-04	}
G_Gs3z5r6	s3z5	0	VALUE =	{	-10*v(s1z5)*v(s4z5)*1.30579E-03	}
G_Gs3z6r6	s3z6	0	VALUE =	{	-10*v(s1z6)*v(s4z6)*2.152883E-03	}
G_Gs3z7r6	s3z7	0	VALUE =	{	-10*v(s1z7)*v(s4z7)*3.549504E-03	}
G_Gs3z8r6	s3z8	0	VALUE =	{	-10*v(s1z8)*v(s4z8)*5.852143E-03	}
G_Gs3z9r6	s3z9	0	VALUE =	{	-10*v(s1z9)*v(s4z9)*9.648553E-03	}
G_Gs3z10r6	s3z10	0	VALUE =	{	-10*v(s1z10)*v(s4z10)*1.590778E-02	}
G_Gs3z11r6	s3z11	0	VALUE =	{	-10*v(s1z11)*v(s4z11)*2.622749E-02	}
G_Gs3z12r6	s3z12	0	VALUE =	{	-10*v(s1z12)*v(s4z12)*4.324182E-02	}
G_Gs3z13r6	s3z13	0	VALUE =	{	-10*v(s1z13)*v(s4z13)*.0712937	}
G_Gs3z14r6	s3z14	0	VALUE =	{	-10*v(s1z14)*v(s4z14)*.1175434	}
G_Gs3z15r6	s3z15	0	VALUE =	{	-10*v(s1z15)*v(s4z15)*.1937964	}
G_Gs3z16r6	s3z16	0	VALUE =	{	-10*v(s1z16)*v(s4z16)*.3195162	}
G_Gs3z17r6	s3z17	0	VALUE =	{	-10*v(s1z17)*v(s4z17)*.5267932	}
G_Gs3z18r6	s3z18	0	VALUE =	{	-10*v(s1z18)*v(s4z18)*.8685351	}
G_Gs3z19r6	s3z19	0	VALUE =	{	-10*v(s1z19)*v(s4z19)*1.431972	}
G_Gs3z20r6	s3z20	0	VALUE =	{	-10*v(s1z20)*v(s4z20)*2.360923	}

*Homogeneous Kinetics Item for No.3 species as An Product at the No.2 Chemical Reaction Ends Here

G_Gs3z1r7	s3z1	0	VALUE =	{	.2*v(s3z1)*v(s3z1)*1.767194E-04	}
G_Gs3z2r7	s3z2	0	VALUE =	{	.2*v(s3z2)*v(s3z2)*2.913611E-04	}
G_Gs3z3r7	s3z3	0	VALUE =	{	.2*v(s3z3)*v(s3z3)*4.803732E-04	}
G_Gs3z4r7	s3z4	0	VALUE =	{	.2*v(s3z4)*v(s3z4)*7.920015E-04	}
G_Gs3z5r7	s3z5	0	VALUE =	{	.2*v(s3z5)*v(s3z5)*1.30579E-03	}
G_Gs3z6r7	s3z6	0	VALUE =	{	.2*v(s3z6)*v(s3z6)*2.152883E-03	}
G_Gs3z7r7	s3z7	0	VALUE =	{	.2*v(s3z7)*v(s3z7)*3.549504E-03	}
G_Gs3z8r7	s3z8	0	VALUE =	{	.2*v(s3z8)*v(s3z8)*5.852143E-03	}
G_Gs3z9r7	s3z9	0	VALUE =	{	.2*v(s3z9)*v(s3z9)*9.648553E-03	}
G_Gs3z10r7	s3z10	0	VALUE =	{	.2*v(s3z10)*v(s3z10)*1.590778E-02	}
G_Gs3z11r7	s3z11	0	VALUE =	{	.2*v(s3z11)*v(s3z11)*2.622749E-02	}
G_Gs3z12r7	s3z12	0	VALUE =	{	.2*v(s3z12)*v(s3z12)*4.324182E-02	}
G_Gs3z13r7	s3z13	0	VALUE =	{	.2*v(s3z13)*v(s3z13)*.0712937	}
G_Gs3z14r7	s3z14	0	VALUE =	{	.2*v(s3z14)*v(s3z14)*.1175434	}
G_Gs3z15r7	s3z15	0	VALUE =	{	.2*v(s3z15)*v(s3z15)*.1937964	}
G_Gs3z16r7	s3z16	0	VALUE =	{	.2*v(s3z16)*v(s3z16)*.3195162	}
G_Gs3z17r7	s3z17	0	VALUE =	{	.2*v(s3z17)*v(s3z17)*.5267932	}
G_Gs3z18r7	s3z18	0	VALUE =	{	.2*v(s3z18)*v(s3z18)*.8685351	}
G_Gs3z19r7	s3z19	0	VALUE =	{	.2*v(s3z19)*v(s3z19)*1.431972	}
G_Gs3z20r7	s3z20	0	VALUE =	{	.2*v(s3z20)*v(s3z20)*2.360923	}

*Homogeneous Kinetics Item for No.3 species as An Product at the No.2 Chemical Reaction Ends Here

G_Gs3z1r8	s3z1	0	VALUE =	{	.2*v(s3z1)*v(s3z1)*1.767194E-04	}
G_Gs3z2r8	s3z2	0	VALUE =	{	.2*v(s3z2)*v(s3z2)*2.913611E-04	}
G_Gs3z3r8	s3z3	0	VALUE =	{	.2*v(s3z3)*v(s3z3)*4.803732E-04	}
G_Gs3z4r8	s3z4	0	VALUE =	{	.2*v(s3z4)*v(s3z4)*7.920015E-04	}
G_Gs3z5r8	s3z5	0	VALUE =	{	.2*v(s3z5)*v(s3z5)*1.30579E-03	}
G_Gs3z6r8	s3z6	0	VALUE =	{	.2*v(s3z6)*v(s3z6)*2.152883E-03	}
G_Gs3z7r8	s3z7	0	VALUE =	{	.2*v(s3z7)*v(s3z7)*3.549504E-03	}
G_Gs3z8r8	s3z8	0	VALUE =	{	.2*v(s3z8)*v(s3z8)*5.852143E-03	}
G_Gs3z9r8	s3z9	0	VALUE =	{	.2*v(s3z9)*v(s3z9)*9.648553E-03	}
G_Gs3z10r8	s3z10	0	VALUE =	{	.2*v(s3z10)*v(s3z10)*1.590778E-02	}
G_Gs3z11r8	s3z11	0	VALUE =	{	.2*v(s3z11)*v(s3z11)*2.622749E-02	}
G_Gs3z12r8	s3z12	0	VALUE =	{	.2*v(s3z12)*v(s3z12)*4.324182E-02	}
G_Gs3z13r8	s3z13	0	VALUE =	{	.2*v(s3z13)*v(s3z13)*.0712937	}

```

G_Gs3z14r8  s3z14 0 VALUE = { .2*v(s3z14)*v(s3z14)*.1175434 }
G_Gs3z15r8  s3z15 0 VALUE = { .2*v(s3z15)*v(s3z15)*.1937964 }
G_Gs3z16r8  s3z16 0 VALUE = { .2*v(s3z16)*v(s3z16)*.3195162 }
G_Gs3z17r8  s3z17 0 VALUE = { .2*v(s3z17)*v(s3z17)*.5267932 }
G_Gs3z18r8  s3z18 0 VALUE = { .2*v(s3z18)*v(s3z18)*.8685351 }
G_Gs3z19r8  s3z19 0 VALUE = { .2*v(s3z19)*v(s3z19)*1.431972 }
G_Gs3z20r8  s3z20 0 VALUE = { .2*v(s3z20)*v(s3z20)*2.360923 }

```

*Homogeneous Kinetics Item for No.3 species as An Product at the No.2 Chemical Reaction Ends Here

```

G_Gslz1r9   slz1 0 VALUE = { -.2*v(s3z1)*v(s3z1)*1.767194E-04 }
G_Gslz2r9   slz2 0 VALUE = { -.2*v(s3z2)*v(s3z2)*2.913611E-04 }
G_Gslz3r9   slz3 0 VALUE = { -.2*v(s3z3)*v(s3z3)*4.803732E-04 }
G_Gslz4r9   slz4 0 VALUE = { -.2*v(s3z4)*v(s3z4)*7.920015E-04 }
G_Gslz5r9   slz5 0 VALUE = { -.2*v(s3z5)*v(s3z5)*1.30579E-03 }
G_Gslz6r9   slz6 0 VALUE = { -.2*v(s3z6)*v(s3z6)*2.152883E-03 }
G_Gslz7r9   slz7 0 VALUE = { -.2*v(s3z7)*v(s3z7)*3.549504E-03 }
G_Gslz8r9   slz8 0 VALUE = { -.2*v(s3z8)*v(s3z8)*5.852143E-03 }
G_Gslz9r9   slz9 0 VALUE = { -.2*v(s3z9)*v(s3z9)*9.648553E-03 }
G_Gslz10r9  slz10 0 VALUE = { -.2*v(s3z10)*v(s3z10)*1.590778E-02 }
G_Gslz11r9  slz11 0 VALUE = { -.2*v(s3z11)*v(s3z11)*2.622749E-02 }
G_Gslz12r9  slz12 0 VALUE = { -.2*v(s3z12)*v(s3z12)*4.324182E-02 }
G_Gslz13r9  slz13 0 VALUE = { -.2*v(s3z13)*v(s3z13)*.0712937 }
G_Gslz14r9  slz14 0 VALUE = { -.2*v(s3z14)*v(s3z14)*.1175434 }
G_Gslz15r9  slz15 0 VALUE = { -.2*v(s3z15)*v(s3z15)*.1937964 }
G_Gslz16r9  slz16 0 VALUE = { -.2*v(s3z16)*v(s3z16)*.3195162 }
G_Gslz17r9  slz17 0 VALUE = { -.2*v(s3z17)*v(s3z17)*.5267932 }
G_Gslz18r9  slz18 0 VALUE = { -.2*v(s3z18)*v(s3z18)*.8685351 }
G_Gslz19r9  slz19 0 VALUE = { -.2*v(s3z19)*v(s3z19)*1.431972 }
G_Gslz20r9  slz20 0 VALUE = { -.2*v(s3z20)*v(s3z20)*2.360923 }

```

*Homogeneous Kinetics Item for No.1 species as An Reactant at the No.2 Chemical Reaction Ends Here

```

G_Gs4z1r10  s4z1 0 VALUE = { -.2*v(s3z1)*v(s3z1)*1.767194E-04 }
G_Gs4z2r10  s4z2 0 VALUE = { -.2*v(s3z2)*v(s3z2)*2.913611E-04 }
G_Gs4z3r10  s4z3 0 VALUE = { -.2*v(s3z3)*v(s3z3)*4.803732E-04 }
G_Gs4z4r10  s4z4 0 VALUE = { -.2*v(s3z4)*v(s3z4)*7.920015E-04 }
G_Gs4z5r10  s4z5 0 VALUE = { -.2*v(s3z5)*v(s3z5)*1.30579E-03 }
G_Gs4z6r10  s4z6 0 VALUE = { -.2*v(s3z6)*v(s3z6)*2.152883E-03 }
G_Gs4z7r10  s4z7 0 VALUE = { -.2*v(s3z7)*v(s3z7)*3.549504E-03 }
G_Gs4z8r10  s4z8 0 VALUE = { -.2*v(s3z8)*v(s3z8)*5.852143E-03 }
G_Gs4z9r10  s4z9 0 VALUE = { -.2*v(s3z9)*v(s3z9)*9.648553E-03 }
G_Gs4z10r10 s4z10 0 VALUE = { -.2*v(s3z10)*v(s3z10)*1.590778E-02 }
G_Gs4z11r10 s4z11 0 VALUE = { -.2*v(s3z11)*v(s3z11)*2.622749E-02 }
G_Gs4z12r10 s4z12 0 VALUE = { -.2*v(s3z12)*v(s3z12)*4.324182E-02 }
G_Gs4z13r10 s4z13 0 VALUE = { -.2*v(s3z13)*v(s3z13)*.0712937 }
G_Gs4z14r10 s4z14 0 VALUE = { -.2*v(s3z14)*v(s3z14)*.1175434 }
G_Gs4z15r10 s4z15 0 VALUE = { -.2*v(s3z15)*v(s3z15)*.1937964 }
G_Gs4z16r10 s4z16 0 VALUE = { -.2*v(s3z16)*v(s3z16)*.3195162 }
G_Gs4z17r10 s4z17 0 VALUE = { -.2*v(s3z17)*v(s3z17)*.5267932 }
G_Gs4z18r10 s4z18 0 VALUE = { -.2*v(s3z18)*v(s3z18)*.8685351 }
G_Gs4z19r10 s4z19 0 VALUE = { -.2*v(s3z19)*v(s3z19)*1.431972 }
G_Gs4z20r10 s4z20 0 VALUE = { -.2*v(s3z20)*v(s3z20)*2.360923 }

```

*Homogeneous Kinetics Item for No.4 species as An Reactant at the No.2 Chemical Reaction Ends Here

```

V_Vs1z21    slz21 0 DC 1
*Boundary Condition at x=infinite for No.1 species Ends Here

```

```

V_Vs2z21    s2z21 0 DC 0
*Boundary Condition at x=infinite for No.2 species Ends Here

```

```

V_Vs3z21    s3z21 0 DC 0
*Boundary Condition at x=infinite for No.3 species Ends Here

```

```

V_Vs4z21    s4z21 0 DC 0
*Boundary Condition at x=infinite for No.4 species Ends Here

```

```

R_Rs1z0      s1z0 s1z1 7.737191E-05
R_Rs2z0      s2z0 s2z1 7.737191E-05
G_Gs1z0r1    s1z0 0
+VALUE={8.944272*(exp(-.5*(V(Ereal)-0)*38.92377)*V(s1z0)-exp(.5*(V(Ereal)-
0)*38.92377)*V(s2z0))}
G_Gouts1z0r2 0 V_Vout_if
+VALUE={1*8.944272*(exp(-.5*(V(Ereal)-0)*38.92377)*V(s1z0)-exp(.5*(V(Ereal)-
0)*38.92377)*V(s2z0))}
*Boundary Condition at x=0 for No.1 species Ends Here

G_Gs2z0r3    s2z0 0
+VALUE={-8.944272*(exp(-.5*(V(Ereal)-0)*38.92377)*V(s1z0)-exp(.5*(V(Ereal)-
0)*38.92377)*V(s2z0))}
*Boundary Condition at x=0 for No.2 species Ends Here

R_Rs3z0      s3z0 s3z1 7.737191E-05
R_Rs4z0      s4z0 s4z1 7.737191E-05
G_Gs3z0r4    s3z0 0
+VALUE={8.944272*(exp(-.5*(V(Ereal)-.3)*38.92377)*V(s3z0)-exp(.5*(V(Ereal)-
.3)*38.92377)*V(s4z0))}
G_Gouts3z0r5 0 V_Vout_if
+VALUE={1*8.944272*(exp(-.5*(V(Ereal)-.3)*38.92377)*V(s3z0)-exp(.5*(V(Ereal)-
.3)*38.92377)*V(s4z0))}
*Boundary Condition at x=0 for No.3 species Ends Here

G_Gs4z0r6    s4z0 0
+VALUE={-8.944272*(exp(-.5*(V(Ereal)-.3)*38.92377)*V(s3z0)-exp(.5*(V(Ereal)-
.3)*38.92377)*V(s4z0))}
*Boundary Condition at x=0 for No.4 species Ends Here

V_Eapp Eapp 0 PWL 0 .6 .25 -.4 .5 .6
+.75      -.4      1      .6
R_if      V_Vout_if 0 8.014244E-02
V_xtoi    xtoi 0 DC 2.113255E-04
E_Eapp    Ereal 0 Eapp 0 1
*.print tran V(V_Eapp) V(R_if) V(V_xtoi);
.save V(Eapp) V(V_Vout_if) V(xtoi);
*.probe V(V_Eapp) V(R_if) V(V_xtoi);
*.watch tran V(R_if);
*.tran .00025 1 0.0 .00025 uic
.tran .00025 1 0.0 .00025
.OPTIONS NUMDGT=6
*.OPT RELTOL=1E-3
.options plotwinsize=0

```

Figure 6. Format of the netlist file "AUTONET.SP" generated by ecNetSim

4.4 Error Checking

To facilitate use and reduce various errors during parameter input, the reaction compiler provides two methods for users to detect and correct errors promptly. The first method is run-time error checking; the second is post-run error checking. The former detects and reports possible input errors immediately during compilation and terminates the program. Users can easily identify and correct errors based on the error messages. Typical detectable errors include:

- (1) Total number of species not specified. The compiler requires users to specify the total number of species involved in the simulation immediately after setting the "method" to CV or CA.
- (2) A species number exceeds the total count. Since the compiler requires consecutive numbering starting from 1, the maximum number should not exceed the total count of species involved in a simulation.
- (3) Missing assignment of initial concentrations or diffusion coefficients. The user may have omitted assigning a concentration or diffusion coefficient for some species.
- (4) Electrode parameters not specified.
- (5) Chronoamperometry and surface events cannot be forced to output current function.
- (6) Simulation time increment exceeds total experiment time.

Post-run error checking writes compilation results to the file INPUT.ATN.CHK (Figure 5). This file's structure mirrors that of INPUT.ATN (Figure 2) but is easier to read. Users can verify whether the content of this file matches that of the original input file. This error-checking method is more thorough and reliable.

4.5 Installation and Operation

Follow these steps to install and run ecNetSim:

(1) Download LTspice — (free software)

(2) Install LTspice.

(3) Locate "LTspice.exe" under the installation directory and create a shortcut named LTspice.lnk in the ecNetSIM main program directory (ecNetSimV6.x_LT.EXE).

(4) Set the option in the input file to Y (set to N if you wish to manually run AUTONET.SP):

[Do you want to run the simulation immediately(Y/N)?(no period)]

Y

(5) Drag the input file "INPUT.ATN" (or any other filename you specified) onto NETSIMV6.x_LT.EXE or its shortcut icon and release the mouse button when prompted to run the simulation (Figure 7). Upon successful execution, the program interface appears as in Figure 8 (ecNetSim interface) and Figure 9 (LTspice plotting interface).

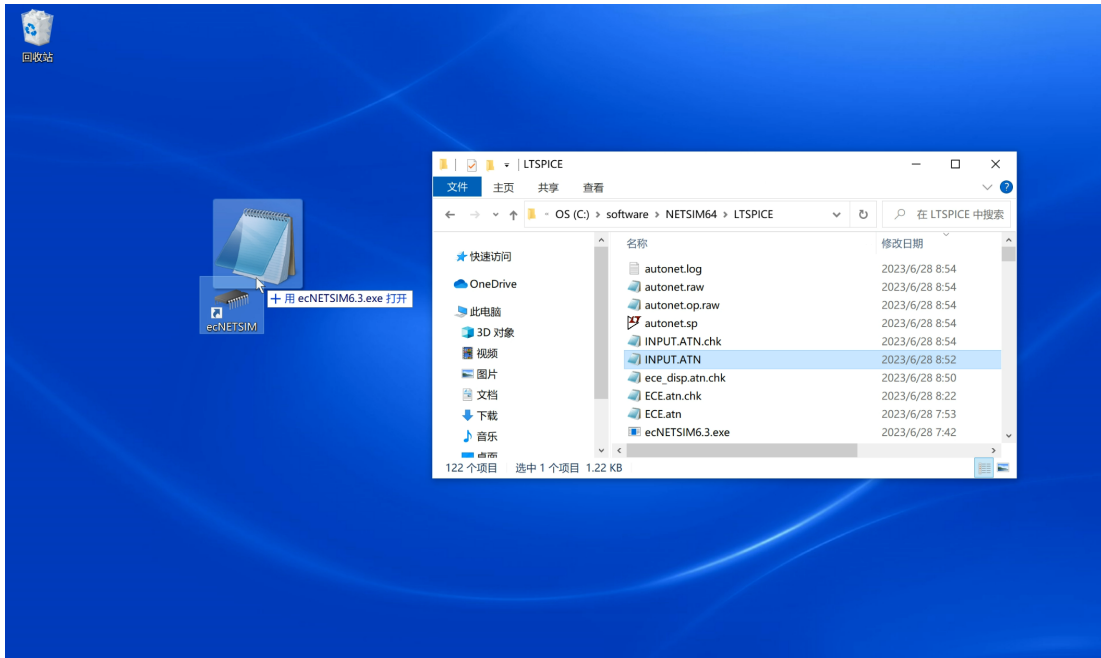


Figure 7. Dragging the input file "INPUT.ATN" onto the ecNetSim shortcut to run the program

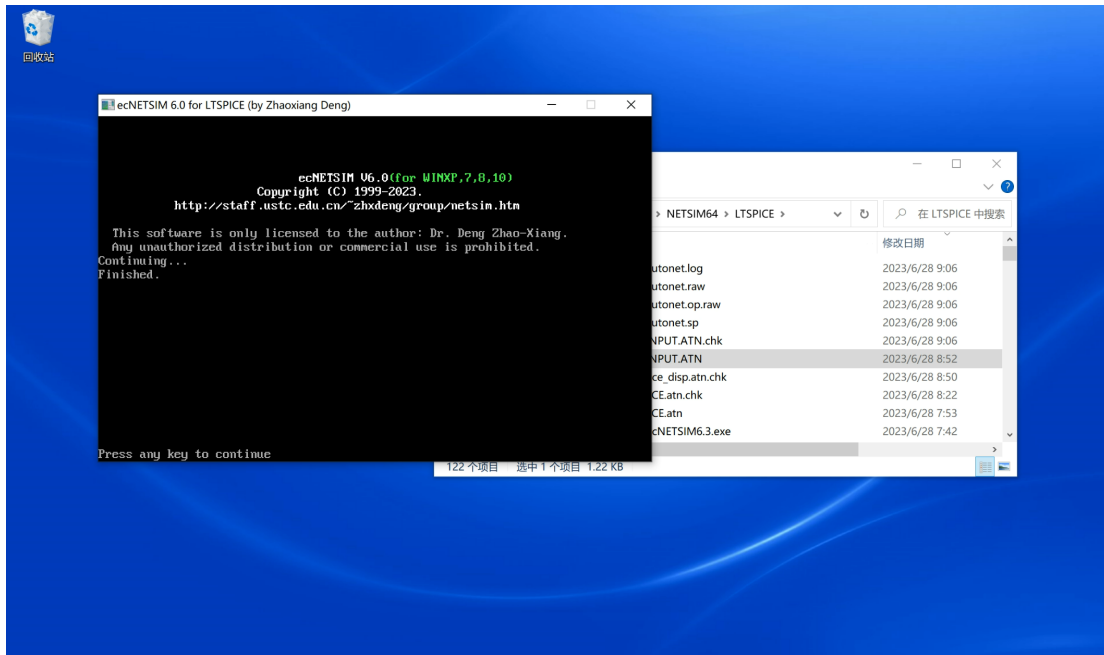


Figure 8. Program interface after ecNetSim has finished running normally

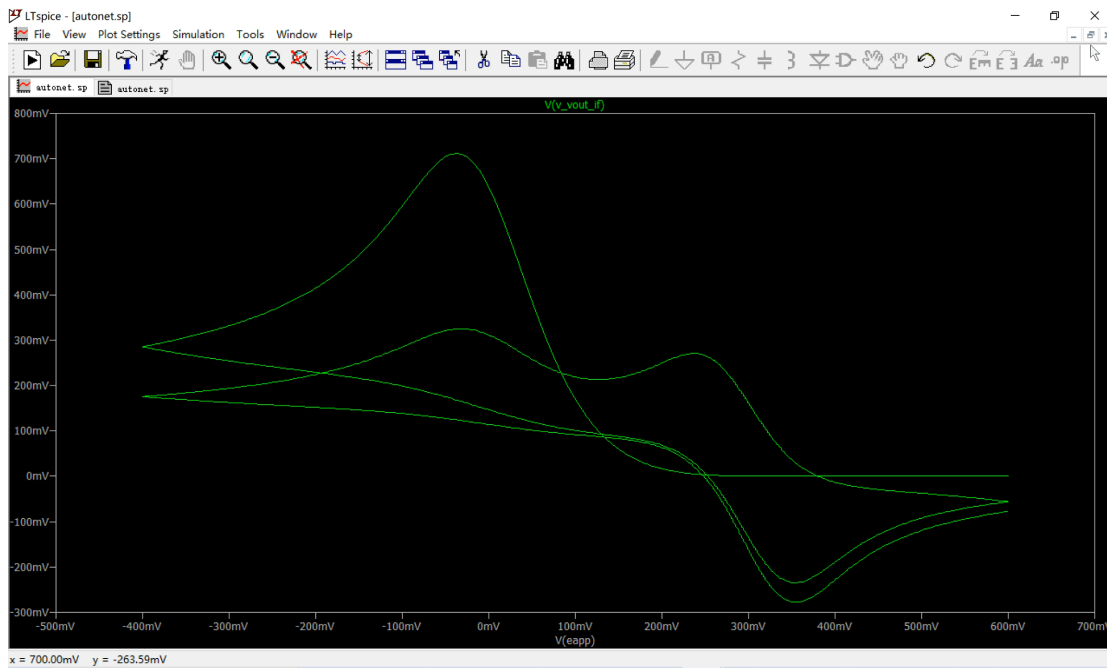


Figure 9. A cyclic voltammetric curve obtained from LTspice simulation based on AUTONET.SP

LTspice download: <https://www.analog.com/en/design-center/design-tools-and-calculators/ltspice-simulator.html>

4.6 Exit

After the software finishes running, press any key to exit or begin a new simulation.