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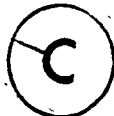
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NETWORK THERMODYNAMICS AND MORPHOGENESIS



by
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Submitted in partial fulfillment
of the Requirements for the degree of
Doctor of Philosophy

Faculty of Graduate Studies
The University of Western Ontario
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ABSTRACT

Network thermodynamics is a method of representing thermodynamic systems as equivalent electrical circuits which allows the application of well-developed techniques of network analysis to thermodynamic problems (Oster, G.F., Perelson, A.S. and Katchalsky, A. 1973. "Network Thermodynamics: Dynamical Modelling of Biophysical Systems."

Q. Rev. Biophys., 6, 1-134). This dissertation covers four aspects.

First, the relevant graph theory, circuit theory including normal tree analysis, and systems theory are summarized to provide a context and working vocabulary for the subsequent sections. Next, a systematic approach is presented for representing thermodynamic systems as equivalent circuits based on dynamical, dimensional, topological and mathematical similarities. Its use is demonstrated by designing an equivalent circuit to represent a primitive autocatalytic reaction-diffusion system (based on the Brusselator) capable of evolving stable asymmetries in the distribution of reactants. This is an example of a morphogenetic system, that is a dynamical chemical system capable of evolving stable changes in structure over time. The resulting equivalent circuit is analyzed using a general circuit simulation language Spice (Dowell, R., Newton, A.R. and Pederson, D.O. 1976. "Spice VAX Version 2X.x User's Guide." Department of Electrical Engineering and Computer Sciences, University of California, Berkeley). Using several different sets of boundary conditions, initial system states and system topologies as examples, the versatility of the

equivalent circuit method is demonstrated. When the most asymmetric topology and open boundary conditions are used, and a non-linear positive feedback loop is used to represent the autocatalytic step, the circuit response shows stable potential differences between distributed subcircuit regions. The final section is a note outlining a method for the sequential synthesis and analysis of a morphogenetic automaton based on network thermodynamics.

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I would like to thank several people who especially aided me in the completion of the dissertation. My husband Irwin supported and encouraged me throughout, particularly with his unwavering conviction that the network approach to the analysis of biological systems has merit. Dr. Suzanne Nuss read and commented upon both the first and final drafts and helped with the mechanics of producing both. Drs. E. Taschdjian, A.L. Szilard, M.H. Sherebrin and J.W. Lorimer suggested revisions to an earlier draft. Dr. Lorimer read and commented upon portions of the revision and intervened on several occasions to allow me time to complete the final draft. Dean Garth Kidd exercised remarkable administrative flexibility, permitting me to finish despite unusual circumstances.

My earlier empirical work on the physiology of maize tissue and suspension cultures and primary root mitochondria performed in the laboratory of Dr. W.G. Hopkins, funded by his research grants, convinced me of the need for some general comparative method for analysis of the resulting data.

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1.1 Introduction

In higher plants, patterns of growth in cells and organs result from an interaction among the genetic instructions, the physical field surrounding the cells and the internal structural field resulting from the morphology of cellular constituents. The genetic program establishes the characteristic configuration of the plant under given environmental circumstances. However, when one looks at the differentiation of individual cells from embryo or meristem, as well as the growth of plant cells in culture, the distinct organismic differences are not particularly apparent. In fact, during the primary events of cell enlargement, cells of higher plants follow a remarkably similar course of increase in cellular constituents and cell division followed by vacuolization. The process of differentiation involving subtle interactions among cells, environment and genome to produce an organism of characteristic form is known as morphogenesis. Historically, the genetic component has been the more accessible, and thus more studied, aspect of the phenomenon. However, biophysical studies of form, particularly those of D'Arcy Thompson (1942) suggest that species differences in morphology can be explained by differences in physical forces and fluxes over space and time, that is, by changes in physical fields.

The cellular physical field may be considered a consequence of the interaction between gene products, assuming all complex structural relations of the cellular constituents are specified by the genetic complement of the cell, and environmental forces and fluxes. If one has two cells taken from different organisms, genetic differences between them may be assessed in two different ways: (1) by directly examining the genetic material; (2) by examining the performance of

some component common to both cells for differences in performance in identical environments. This approach may also be used with cells of the same genetic make-up, but derived from different environments. Genetic differences or differences in gene expression are then inferred from differences of functions in the same environment.

Difficulties arise with these methods in the study of morphogenesis because field effects and interactions among spatially distinct structures and substances within the cell are important and the interactions are combinatorial and non-linear so that a small number of changes propagate over time to large morphogenetic effects. Additionally, many approaches to the study of morphogenesis are descriptive rather than analytical or predictive. Into this class fall the measurements of structural changes in chromosomes, associations between chromosomes, changes in amounts and types of RNA in nucleus and cytoplasm during the course of development, and measurement of enzyme function, levels and substrates over time, etc. For organisms with sizeable aggregations of data on parameters of cellular development--carrot, sycamore, and tobacco cell cultures for example, the patterns of development are described. But using the known genetic and physiological data for these systems to predict the consequences of their interactions on emergent higher levels of organization remains a problem.

The difficulties in assessing and representing multi-level interactions among field effects; transport phenomena and the effects of plant hormones and other variables on cellular differentiation motivated the search for a method with sufficient generality and flexibility to predict and analyze these interactions. Network thermodynamics

meets these criteria for the following reasons:

- 1) It is based on explicit components—the variables and constitutive relations of electrical equivalent networks, the topological relations of orthogonal vector spaces represented by graphs and associated topological matrices, and the properties of general dynamical systems.
- 2) It is topological and independent of specific metric context.
- 3) It allows reduction from many initial physical domains to equivalent electrical circuit representations.
- 4) It allows comparison of heterogeneous data inputs using well-established techniques of network analysis and network modelling.

To develop the methods for analyzing morphogenetic systems using network thermodynamics, a very simple prototype is used. The ways in which it can be analyzed and altered to a system of different topology are discussed below in non-mathematical terms. This provides a basic model of morphogenesis which can eventually be expanded to handle the complexities of biological systems. The basis for representing the prototype as an equivalent circuit is outlined in the subsequent section.

1.2 Description of an Elementary Thermodynamic System

Take a chemical system and partition it arbitrarily into three parts—a volume element, the boundary between the volume element and surroundings, and the surroundings. The volume element is taken to be the most elementary form of a thermodynamic system.

The partitioned chemical system can have in general three primary exchange conditions across the boundary with the surroundings: no ex-

change, movement into the volume from the surroundings, movement from the volume into the surroundings. If no factors but the configuration of the system and its constituents at a given moment cause movements across the boundary, that is, no additional energy is applied to the system, the exchanges are passive. Passive movements of a given substance restrict the net exchange conditions at a given time to two alternatives: no exchange, or flow down a potential gradient (Fig. 1).

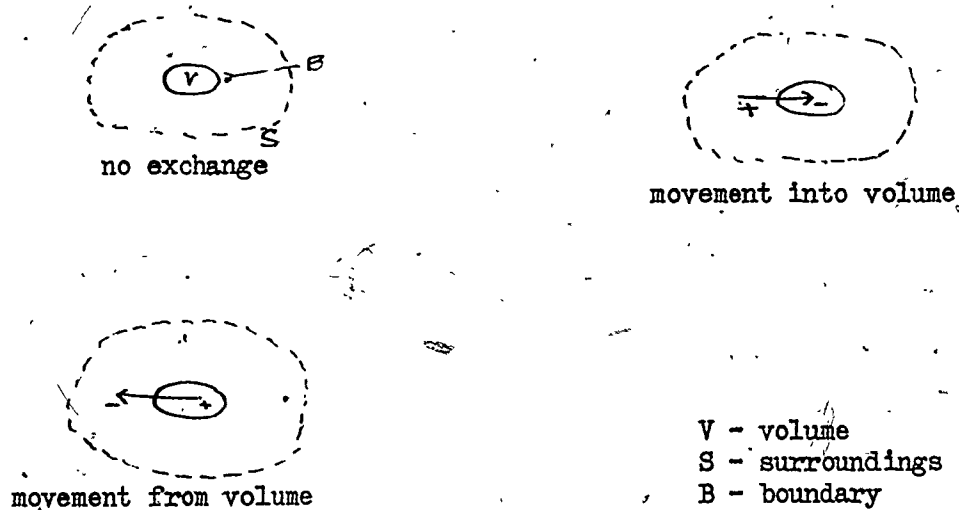


Figure 1

Exchanges can be viewed from two perspectives: the flow or movement across the boundary; or the difference in potential or force between two points. The two processes are independent in the sense that either can initiate change in the other. However, they are also linked or coupled in the passive condition because a change cannot occur in flow without a corresponding change in the associated force, nor can a change of force occur without a corresponding alteration of flow across the boun-

dary. The two coupled variables are represented graphically by a directed branch $\overleftrightarrow{}$, where the signs indicate the direction of the gradient of the force variable, and the arrow indicates the direction of flow.

The passive movement of a substance down a concentration gradient, i.e., diffusion, is only one example of a number of kinds of exchanges which can occur across a volume element boundary. Other force-flow variable pairs are electrical potential-electrical current; temperature-entropy flow; pressure-volume change; and chemical affinity-reaction flow. Each pair will be called a physical domain because each set of variables (conjugate variables) can be studied in its own right independently of the others.

If two or more processes are occurring simultaneously, coupling can occur between flows and forces of different physical domains. For example, a system which has both electrical and diffusion flows occurring simultaneously can have the electrical flow coupled to both diffusion force or potential and electrical potential. At equilibrium no coupling occurs between physical domains (Prigogine, 1967). All forces equal zero, and there are no net flows. But near-to-equilibrium fluctuations in forces and fluxes of several physical domains are non-zero and coupling may occur. If the near-to-equilibrium state is stable, the increase in flow or force in one direction is balanced by those occurring equally in the opposite direction so that the total behavior (trajectory) of the system remains within some boundary. In fact, the fluctuations occurring in a near-to-equilibrium system range from large to small at any given instant (Fig. 2), but their distribution is consistent with the larger or macroscopic behavior of

the system. Note the possibility of large fluctuations of individual components within a macroscopically steady-state system.

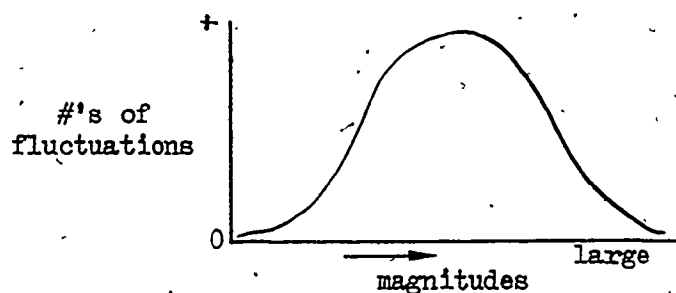


Figure 2. Distribution of Magnitudes of Fluctuations

The condition "near-to-equilibrium" seems at first thought to be restrictive, but in fact it covers a large range of chemical systems, including many biological systems. For example, the notion of homeostasis in physiology is similar to near-to-equilibrium in principle.

In any near-to-equilibrium passive system fluctuations are accompanied by irreversible processes and corresponding increases in entropy. This means that any near-to-equilibrium process in one physical domain must be considered a system coupled between that domain and entropy-temperature changes. Entropy can be regarded as a flow, temperature as a potential variable.

Once two or more physical domains are coupled, the behavior of each individual flow variable becomes a function of all coupled force variables. If one looks at each variable pair in a coupled system, the flow and force variables may not behave as they would in an uncoupled system; direction of positive flow of a given variable can be against its own potential gradient of its own conjugate force variable, providing that the positive magnitude of one or more other

coupled force variables is great enough to create a counter potential gradient. In biological systems, for example, coupling of a flow variable to several forces to produce flow against the potential gradient of a conjugate force is called facilitated diffusion when the process occurs in membrane transport systems.

The configuration of the basic chemical system of volume, boundary and surroundings has been assumed so far. This condition is called a zero-input system. An alternative way of viewing the system is to set the initial conditions to zero (or some arbitrary state) with respect to variables of interest, called zero-state. One may then introduce to some part(s) of the system, known as ports, measured inputs (an active process) as either force or flow variables, and observe force and flow changes between surroundings and volume element. In this case the system is open and no longer near-to-equilibrium.

1.3 Structural Change in an Elementary Thermodynamic System

Generally, the increase in entropy in a chemical system is associated with increasing homogeneity in the distribution of substances throughout. However, in non-equilibrium systems, the increase in entropy is not incompatible with increase in structural complexity of subsystems. There are two basic ways in which increase in structural complexity interacts with increasing entropy. First, in the context again of the basic system, the entropy produced within the volume can be transported to the surroundings against the potential gradient when entropy flow is coupled with variable changes of other physical domains. Although the entropy increase occurs for the system as a whole in accordance with the 2nd Law of Thermodynamics, the

distribution of entropy within the system is not homogeneous.

The second way in which increase in structural complexity can occur while entropy increases is in the formation of "dissipative structures" in open, far-from-equilibrium systems. (Cf., Glansdorff and Prigogine, 1971; Nicolis and Prigogine, 1977.) If the system is poised at a certain transition point, a very small change in a variable can destabilize the entire system and cause it to eventually assume a new configuration compatible with a new macroscopic steady state. Or several small perturbations can resonate to produce a summative effect larger than any of the individual components. Perturbations of sufficient magnitude can provide the necessary driving force. Actually, the system at the critical point can be either active or passive (although active processes may have been necessary to bring it to the transition point) and structural changes beyond that point can involve only passive fluxes and forces associated with increasing entropy due only the configuration of the system components.

Changes in structure or morphology of the volume element can be separated into two general classes:

- 1) increase or decrease in total volume;
- 2) creation or disappearance of stable asymmetries in the distribution of potentials and flows within the volume.

The first class is governed by changes in potentials and flows between the volume and the surroundings. The second class involves creation of stable asymmetries by partitioning the volume element into sub-volumes with more or less distinct boundaries. The exchanges between the sub-volumes are governed by the same considerations as those governing

exchanges between volume and surroundings. The four types of structural changes are the most primitive examples of morphogenesis. The disappearance of stable asymmetries means that forces and flows between the surroundings and volume can no longer be distinguished, that is, the boundary disappears.

The original volume element was assumed to be internally homogeneous with respect to any given variable. If rules are given for dividing the volume element into two (or more) parts again meeting some specified homogeneity condition when some threshold value of change in size or steady state asymmetry of a force or flow is reached, a new configuration occurs with the spatial system now partitioned into two (or more) distinct volume elements, each with a distinct boundary that separates it from the surroundings and the other volume element(s). With the new configuration, the possibilities for exchanges between different parts of the system are increased. For example, the condition "no net exchange" becomes no net exchange between surroundings and volume 1, surroundings and volume 2, and between volume 1 and volume 2.

If a single flow variable f and its conjugate potential variable Y are taken to vary between different parts of a two volume system, the possible interactions can be enumerated in a pair of matrices:

$$\begin{array}{c}
 \begin{array}{ccc}
 V_1 f^- & V_2 f^- & S f^- \\
 \hline
 V_1 Y^+ & 0 & V_1 Y^+ V_2 f^- \quad V_1 Y^+ S f^- \\
 V_2 Y^+ & V_2 Y^+ V_1 f^- & 0 \quad V_2 Y^+ S f^- \\
 S Y^+ & S Y^+ V_1 f^- & S Y^+ V_2 f^- \quad 0
 \end{array}
 \qquad
 \begin{array}{ccc}
 V_1 f^+ & V_2 f^+ & S f^+ \\
 \hline
 V_1 Y^- & 0 & V_1 Y^- V_2 f^+ \quad V_1 Y^- S f^+ \\
 V_2 Y^- & V_2 Y^- V_1 f^+ & 0 \quad V_2 Y^- S f^+ \\
 S Y^- & S Y^- V_1 f^+ & S Y^- V_2 f^+ \quad 0
 \end{array}
 \end{array}$$

where V_1 is volume 1, V_2 is volume 2, S is surroundings, f is the flow variable, Ψ is the potential or force variable. Exchanges between volume 1 and volume 2 are diagrammed in Figure 3.



Figure 3

Since each volume element is assumed to be homogeneous, there are no net flows or forces operating internally, and the appropriate matrix entry is zero.

Even in a simple two volume system, if several physical domains are coupled and several substances are moving across boundaries, the number of possible combinations of exchange is large. Generally, effects of interest can be considered as a function of a smaller number of factors as an approximation.

This discussion is based on some of the notions of irreversible thermodynamics which have been developed in a number of more technical presentations (cf. Katchalsky and Curran, 1965; Prigogine, 1967; Glansdorff and Prigogine, 1970; Nicolis and Prigogine, 1977; Prigogine, 1980; De Groot and Mazur, 1962; Meixner and Reik, 1959).

1.4 Electrical Equivalent Circuits of Thermodynamic Systems

If one wishes to examine behavior of a thermodynamic system over

an interval of time, there are three basic ways to proceed. First, one can measure the system parameters directly over time. This may not be possible in complex systems, systems with subcomponents inaccessible to direct measurement (often the case with biological systems in vitro), or in analysis of essentially hypothetical systems such as the "Brusselator" reaction-diffusion system (see section 4). Alternatively, the system can be described mathematically with a set of equations which can be solved exactly or approximated; or it can be simulated with an equivalent system which is more easily monitored. One equivalent system which is widely used by engineers to simulate behavior of other systems is the electrical equivalent circuit.

The basis for equivalence is first, the underlying properties shared by dynamical systems, that is systems which are described by both position and velocity.

The second basis for equivalence is the dimensional similarity between electrical variables and variables from other physical domains. For comparison, the more general terms for variables—effort (force or potential) and flow—are used to maintain the distinction between generalized variables and any particular variables of a physical domain. (Dimensional analysis of variables of physical domains is given in section 3). If two variables from different physical domains can be expressed in comparable units of length, mass or charge, and time, they are considered to be equivalent. For example, the dimension of electrical current is $t^{-1}q$ (or 1/unit time multiplied by unit charge); the dimension of diffusion flow is $t^{-1}m$ (or 1/unit time multiplied by unit mass). For the purpose of constructing an equivalent circuit, an analogy is made between electrical charge and mass, called the mass-

capacitance analogy, charge being a capacitance variable. The same process is applied to diffusion equivalent dimensions for voltage, current and flux linkage—the basic electrical network variables.

The third basis for equivalence is topological. Interconnections between branches in the equivalent circuit bear the same logical relationships as interconnections of elements and functions in the system being modelled.

The fourth basis for equivalence is mathematical. Given a mathematical equation or set of equations, with suitable transformations to ensure dimensional equivalence, an electrical network can be synthesized directly from the equations. Or starting from the opposite end of the process, given an electrical circuit, a set of state equations can be written from the circuit and solved analytically.

Computer programs for simulation of electrical circuits allow the analysis of circuit behavior directly from parameter settings (values of capacitance, resistance, inductance, impedance or admittance) and circuit topology (the way the circuit element branches are directed and connected), and sources of current or voltage applied to the circuit, along with any internal sources. By exploiting the bases for equivalence between thermodynamic systems and electrical networks, circuit simulation programs can be used to model thermodynamic systems.

1.5 Summary of Subsequent Sections

Subsequent sections of this paper give detailed discussions and literature references. Section 2 outlines the pertinent background definitions and equations from graph theory and electrical network analysis. It is not necessary to read this section for continuity of pre-

resentation. Section 3 discusses the history of the combination of circuit theory and thermodynamics called network thermodynamics. The details of bases for constructing equivalent circuits, analogies between thermodynamic field equations, Maxwell's equations and equivalent circuits complete the section.

Section 4 presents an electrical equivalent circuit simulation of the Brusselator reaction-diffusion system. This system has been of theoretical interest to biologists because it is the simplest autocatalytic reaction system capable in principle of generating stable spatial inhomogeneities in concentrations of intermediate substances.

Section 5 outlines a scheme for the construction of a dynamical automaton to model the process of morphogenesis based on both structural and parameter changes in an initial network.

2. Network Analysis

2.1, Introduction

Networks representing thermodynamic systems can be divided and analyzed in several ways. This section gives basic definitions and relations for the following areas: The underlying topological structure is represented by a directed graph. Ways of partitioning the directed graph are represented by matrices. Overlying the graph topology are the variables and constitutive relations associated with the branches which define the equivalent circuit. Analogous to the partitioning of the directed graph are the topological methods of analysis based on Kirchoff's Laws and Tellegen's theorem. Finally, state space analysis of networks, the normal tree method of writing state equations, and computerized circuit simulators are discussed.

2.2 Concepts Describing a Directed Graph

This section is drawn from presentations of Chen (1976), Bryant (1967), Deo (1974) and Stern (1965).

2.2.1 A connected directed graph (interchangeably called network or circuit) consists of a set of nodes, V and a set of directed branches, E , connecting ordered pairs of nodes.

2.2.2 A branch (i, j) is directed from node i to node j , or incident with nodes i and j .

2.2.3 The degree of a node n_i is the number of branches incident with it. Since each branch is incident with two nodes, it contributes 2 to the sum of the degrees of the nodes for undirected graphs. Hence, $\sum_{i=1}^n d_i = 2b$, where d denotes degree, b denotes branch.

Outgoing and incoming degrees. The outgoing degree of node i is the number $d^+(i)$ of branches having node i as their initial node, i.e., branches directed from the node; the number $d^-(i)$ of branches having node i as their terminal node, i.e., branches directed to the node, is called the incoming degree of node i ; and $d(i) = d^+(i) + d^-(i)$. The number of branches in a directed graph is related to the degrees of its nodes by the following equation:

$$b = \sum_i d^+(i) = \sum_i d^-(i)$$

2.2.4 A subgraph of directed graph $G(V, E)$ is a graph $G_s(V_s, E_s)$ in which V_s and E_s are subsets of V and E respectively. If $V_s = V$, the subgraph is called a spanning subgraph of G . If V_s of G_s is empty, the subgraph is a null subgraph.

2.2.5 Isomorphism. Two graphs are isomorphic if there is one-to-one correspondence between the elements of their node sets and a one-to-one correspondence between the elements of their branch sets, and corresponding branches are incident into and out of corresponding nodes.

2.2.6 Path: an open branch sequence (that is, branch $i_1 \neq i_k$) in which the branches are distinct, appearing only once in the sequence, and all the nodes are distinct.

2.2.7 Loop: a closed branch sequence (branch $i_1 = i_k$) in which the branch sequence is distinct and the nodes are distinct.

2.2.8 Cut Set. A cut set of a connected graph consists of the minimal set of branches whose removal disconnects the graph.

2.2.9 Components and connectedness of graphs. A graph is connected if there is at least one branch between each pair of nodes.

Otherwise the graph is disconnected. A connected graph has one component (maximally connected subgraph); a disconnected graph has two or more components.

2.2.10 Spanning Tree. A spanning tree of a connected graph is a subgraph containing all nodes of the graph, but no loops. All spanning trees of a connected graph of n nodes contain $n - 1$ branches. The number of spanning trees of a graph is:

$$T = \det (\underline{A} \cdot \underline{A}^T),$$

where \underline{A} is the incidence matrix, and \underline{A}^T is the transposed incidence matrix.

2.2.11 Binet-Cauchy Theorem. The number of spanning trees can be computed using the Binet-Cauchy Theorem: If \underline{Q} and \underline{R} are $k \times m$ and $m \times k$ matrices, respectively, with $k \leq m$, the $\det(\underline{Q} \cdot \underline{R}) =$ sum of the product of the major determinants of \underline{Q} and \underline{R} .

2.2.12 Chord. A chord is a branch whose addition to a spanning tree produces a unique (fundamental) loop.

2.2.13 Co-tree: the complement of a spanning tree whose branches are composed of chords.

2.2.14 Rank. The rank r of a graph with n nodes and k components is $r = n - k$. The rank of a graph is equal to the number of branches in a spanning tree for a connected graph.

2.2.15 Nullity. Nullity m of a graph with b branches, n nodes and k components is $m = b - n + k (= b - r)$.

A graph has $m = 0$ iff (if and only if)

it contains no loops, and $m = 1$ iff it contains a single loop. The nullity is equal to the number of chords in a graph, and therefore to the number of fundamental loops in the graph.

The sum of rank and nullity for a graph equals the number of branches in the graph.

2.2.16 Basis: the number of independent elements (vectors) or dimensions spanning a graph. For the loop space of a graph (composed of all fundamental loops of the graph), the basis is the number of branches in a spanning tree. For the cut space (composed of all the fundamental cut sets of the graph), the basis is the number of chords. All other elements can be derived as linear combinations of the basis elements. The number of elements in the basis of one spanning tree is the same as in another spanning tree, and the number of possible bases for the graph is the number of spanning trees. The case for the cut space is equivalent.

2.3 Set-Theoretic Binary Operations on Graphs

2.3.1 Union (sum graph) $G_1 \cup G_2$: If $G_1(V_1, E_1)$ and $G_2(V_2, E_2)$ are two subgraphs of graph $G(V, E)$, then $G_1 \cup G_2$ is a subgraph of G with node set $V_1 \cup V_2$ and branch set $E_1 \cup E_2$.

2.3.2 Intersection graph $G_1 \cap G_2$: the subgraph with node set $V_1 \cap V_2$ and branch set $E_1 \cap E_2$, that is, nodes and branches which are in both G_1 and G_2 .

2.3.3 Difference $G_1 - G_2$: consists of all graph elements which are in G_1 but not in G_2 .

2.3.4 Ring Sum $G_1 \oplus G_2$: is the difference between the union and

intersection graphs: $G_1 \oplus G_2 = (G_1 \cup G_2) - (G_1 \cap G_2)$.

2.4 Matrices Representing Directed Graphs

2.4.1 Incidence Matrices.

The augmented incidence matrix \underline{A}_a of a graph is a matrix of order $n \times b$ with entries of $\pm 1, 0$ defined as follows:

$a_{jk} = +1$ if branch k is incident with node j and oriented away from it.

$a_{jk} = -1$ if branch k is incident with node j and oriented towards it.

$a_{jk} = 0$ if branch k is not incident with node j .

The incidence matrix is not defined for graphs containing self-loops (branches which are incident on to and away from the same node). The rank of \underline{A}_a is $n - k$, where k is the number of components of the graph. \underline{A}_a is a singular matrix, i.e., its determinant is equal to zero, or equivalently, not all rows are independent.

The reduced incidence matrix \underline{A} (hereafter referred to simply as incidence matrix) is formed by dropping any row of \underline{A}_a (equivalent to dropping a reference node). The incidence matrix \underline{A} is a non-singular square matrix with rank $(n - 1)$, order $(n - 1) \times b$, and determinant equal to ± 1 . \underline{A} can be partitioned into two submatrices: \underline{A}_t consisting of $n - 1$ columns corresponding to the branches of a spanning tree, and \underline{A}_c where columns are the remaining $(b - n + 1)$ chords:

$$\underline{E} = [\underline{A}_t, \underline{A}_c]$$

$$\underline{E}^T = [-\underline{A}_t^{-1}, \underline{A}_c]$$

2.4.2 Loop Matrices.

The loop matrix \underline{B}_a is a matrix of order $m \times b$ where m = number of

loops in a graph; and rank is $(b - n + k)$ with columns equal to the number of branches, rows equal to the number of loops in the graph. Entries in the matrix are $\pm 1, 0$ defined as follows:

$b_{jk} = +1$ if branch k is incident with loop j with orientations coinciding.

$b_{jk} = -1$ if branch k is incident with loop j and their orientations are opposite.

$b_{jk} = 0$ if branch k and loop j are not incident.

The orientation of a loop is an arbitrarily assigned direction (clockwise or counterclockwise); and each loop in a graph may be assigned an orientation independently of all other loops in the same graph.

A fundamental loop matrix \underline{B}_f is a submatrix of \underline{B}_a of order $(b - n + 1) \times b$ with loops composed of the spanning trees and associated chords of the graph. The orientations of the fundamental loops are chosen to coincide with the direction of the chords. If the loop branches are partitioned with the chord branches arranged to form the first m columns of \underline{B}_f , the fundamental loop matrix is written:

$$\underline{B}_f = \left[\underline{I}_m, \underline{F} \right]$$

where $m = b - n + 1$, and \underline{I}_m is the basis identity matrix of order $(b - n + 1) \times (b - n + 1)$, and \underline{F} is a $(b - n + 1) \times (n - 1)$ submatrix composed of the remaining tree branches.

An identity matrix is a matrix whose diagonal elements are $+1$'s and off-diagonal elements are zeros.

2.4.4 Cut-Set Matrices.

A cut-set matrix \underline{Q}_a is a cut by branch matrix of order $q \times b$

with rows equal to the number of cuts and columns equal to the number of branches, with

$q_{ik} = +1$ if the orientation of the branch agrees with the orientation of the cut.

$q_{ik} = -1$ if the orientation of the branch is opposite that of the cut.

$q_{ik} = 0$ if the branch is not in the cut.

A fundamental cut set matrix Q_f has cuts each of which contain only one branch of a unique spanning tree, with the remaining branches chords. The f -cut set orientation is chosen to correspond to that of the associated spanning tree branch. The column branches of the Q_f matrix can be partitioned into spanning tree and chord edges with spanning tree branches forming an identity submatrix I_f , of order $(n - 1) \times (n - 1)$, the rank of which is equal to the number of independent cuts in Q_f , and the remaining edges forming a submatrix $-F^T$ of order $(n - 1) \times (b - n + 1)$:

$$Q_f = \begin{bmatrix} -F^T & I_f \end{bmatrix}.$$

The cut space is orthogonal to the loop space.

2.4.5 An adjacency or relational matrix C of a connected graph is a node by node matrix where:

$c_{ij} = 1$ if a branch is directed from node i to node j .

$c_{ij} = 0$ otherwise.

Self-loops have a value of +1 on the main diagonal.

2.5 Variables and Constitutive Relations for Elements of Interpreted Directed Graphs

2.5.1 The branches of directed graphs are interpreted in electrical networks as one- or multi-port or two or more terminal elements—resistors, inductors, capacitors or sources, which may be active or passive, time varying or time invariant, linear or non-linear. Each of type of element is described by a constitutive relation between a current vector and voltage vector. Voltage and current vectors are members of the more general class of effort and flow vectors. Since applications here cover several physical domains, the general terms effort, e , and flow, f , momentum, p , and displacement, q , will be used when no particular physical domain is being considered.

2.5.2 Vector variables are described by the following relations:

$$e = dp/dt$$

$$f = dq/dt$$

$$p = \int e(t) dt$$

$$q = \int f(t) dt$$

$$\underline{e}_s(t), f = 0$$

$$\underline{f}_s(t), e = 0$$

where $\underline{e}_s(t)$ and $\underline{f}_s(t)$ are source vectors.

2.5.3 For the independent flow source terminal, flow of a one-port element is always equal to some function of time regardless of the value of the effort across its terminals. For the independent effort source, terminal effort of a one-port element is always equal

to some function of time regardless of the value of the flow through its terminals.

2.5.4 Reference directions for branch flows and efforts (Chua, 1969): By convention, positive power is taken to flow into a black box network element (branch). This condition is satisfied whenever the flow variable is chosen to enter the specified positive terminal and leave the negative terminal. The sign of the effort difference between the branch terminals is opposite to that of the direction of flow. That is, if flow through a branch element from node a to b is positive $f(a \rightarrow b)$, potential across the connecting branch is $e(b \rightarrow a)$ and the power, $p(t) = e(t) \cdot f(t) > 0$.

2.5.5 Constitutive relations describing branch elements: Constitutive relations are state equations giving functional relations between effort and flow variables for network branch elements as a generalized form of Ohm's Law.

2.5.6 Resistor Elements: For linear resistor one ports:

$$e = R f \text{ (Ohm's Law), } R = \text{resistance;}$$

$$f = 1/R e \text{ or } f = G e, G = \text{conductance.}$$

For non-linear resistors the $e - f$ characteristic curve is not a straight line, and may have either positive or negative slope (Chua, 1969).

Effort-controlled resistors: $f = f(e)$. Flow is a single-valued function of effort, but not vice versa.

Flow-controlled resistors: $e = e(f)$. Effort is a single-valued function of flow, but not vice versa.

A strictly monotonically increasing resistor is both effort and

flow controlled and can be described by either $f = f(e)$ or $e = e(f)$. A multi-valued resistor is neither effort-controlled nor flow-controlled.

Incremental parameter forms of constitutive relations for network elements (Stern, 1964) are used in the state variable (time-domain) approach to network analysis of non-linear networks. The incremental parameter constitutive relations (Jacobian matrix) for n-port resistor elements are:

$$\frac{\partial e_R}{\partial f_R} = \underline{R}(t, f_R) \triangleq \begin{bmatrix} R_{\bar{t}\bar{t}} & R_{\bar{t}t} \\ R_{t\bar{t}} & R_{tt} \end{bmatrix},$$

where subscripts t and \bar{t} refer to tree branches and chords, respectively, \triangleq indicates definition. Submatrices $R_{\bar{t}\bar{t}}$, $R_{\bar{t}t}$, $R_{t\bar{t}}$ and R_{tt} represent

$$\frac{\partial e_t}{\partial f_t}, \quad \frac{\partial e_{\bar{t}}}{\partial f_{\bar{t}}}, \quad \frac{\partial e_{\bar{t}}}{\partial f_t}, \quad \text{and} \quad \frac{\partial e_t}{\partial f_{\bar{t}}}.$$

The hybrid form of the incremental resistance in terms of mixed variables is:

$$\frac{\partial (f_{\bar{t}}, e_t)}{\partial (e_{\bar{t}}, f_t)} = \underline{H}(t, e_{\bar{t}}, f_t) \triangleq \begin{bmatrix} H_{\bar{t}\bar{t}} & H_{\bar{t}t} \\ H_{t\bar{t}} & H_{tt} \end{bmatrix}$$

Incremental conductance (reciprocal resistance) is:

$$\frac{\partial f_R}{\partial e_R} = \underline{R}^{-1} = \underline{G}(t, e_R) \triangleq \begin{bmatrix} G_{\bar{t}\bar{t}} & G_{\bar{t}t} \\ G_{t\bar{t}} & G_{tt} \end{bmatrix}$$

2.5.7 Capacitance Elements: The constitutive equations for linear capacitor one-ports are:

$$q = C e,$$

$$f(t) = C (de(t)/dt).$$

A linear capacitor is completely characterized by these relations.

For a non-linear capacitor the entire $e \cdot q$ curve is required to characterize the element:

Effort-controlled capacitor: $q = q(e)$;

Displacement-controlled capacitor: $e = e(q)$.

For the effort-controlled one-port capacitor, flow entering the capacitor can be expressed as incremental capacitance (Chua, 1969):

$$f(t) = \frac{dq(t)}{dt} \cong \frac{dq(e)}{de} \cdot \frac{de(t)}{dt},$$

or

$$f(t) = C(e(t)) \frac{de(t)}{dt},$$

where

$$C(e) \equiv dq(e)/de.$$

Incremental parameter constitutive relations for n -port capacitors, where $e_{\bar{t}}$, $q_{\bar{t}}$ are co-tree vectors, e_t and q_t are tree vectors, are as follows (Stern, 1964):

$$\frac{\partial q_C}{\partial e_C} = c(t, e_C) \triangleq \begin{bmatrix} C_{\bar{t}\bar{t}} & C_{\bar{t}t} \\ C_{t\bar{t}} & C_{tt} \end{bmatrix},$$

where

$$q_C = q_C(t, e_C) = \begin{bmatrix} q_{\bar{t}}(t, e_{\bar{t}}, q_t) \\ e_t(t, e_{\bar{t}}, q_t) \end{bmatrix}.$$

The hybrid capacitance matrix in terms of mixed variables

$$q_{\bar{t}} = q_{\bar{t}}(t, e_{\bar{t}}, q_t),$$

$$e_t = e_t(t, e_{\bar{t}}, q_t),$$

is

$$\frac{\partial (q_{\bar{t}}, e_t)}{\partial (e_{\bar{t}}, q_t)} = K(t, e_{\bar{t}}, q_t) \triangleq \begin{bmatrix} K_{\bar{t}\bar{t}} & K_{\bar{t}t} \\ K_{t\bar{t}} & K_{tt} \end{bmatrix}.$$

If

$$e_{\bar{t}} = e_{\bar{t}}(t, q_{\bar{t}}, q_t),$$

$$e_t = e_t(t, q_{\bar{t}}, q_t),$$

the incremental elastance form (reciprocal of capacitance) is:

$$\frac{\partial e_c}{\partial q_c} = c^{-1} = S(t, q_c) \triangleq \begin{bmatrix} S_{\bar{t}\bar{t}} & S_{\bar{t}t} \\ S_{t\bar{t}} & S_{tt} \end{bmatrix}.$$

2.5.8 Inductance Elements: The constitutive relation for a one-port linear inductor is

$$p = L f, \quad e(t) = L(df(t)/dt),$$

where L is the slope of a straight line characterizing the behavior of the element. For non-linear inductors, the $f \cdot p$ curve is not a straight line, and to characterize the element the entire $f \cdot p$ curve must be given (Chua, 1969):

$$\text{Flow-controlled inductor: } p = p(f);$$

$$\text{Momentum (flux) controlled inductor: } f = f(p).$$

For the flow-controlled one-port inductor, effort across the inductor branch is expressed as the incremental inductance:

$$e(t) = \frac{dp(t)}{dt} = \frac{dp(f)}{df} \cdot \frac{df(t)}{dt},$$

or

$$e(t) = L f(t) \left(\frac{df(t)}{dt} \right)$$

where

$$L(f) \equiv dp(f)/df.$$

Incremental parameter constitutive relations for n-port inductors are as follows, where $p_{\bar{t}}$ and $f_{\bar{t}}$ are co-tree vectors, p_t and f_t are tree vectors:

$$\frac{\partial p_L}{\partial f_L} = \underline{L}(t, f_L) \triangleq \begin{bmatrix} L_{\bar{t}\bar{t}} & L_{\bar{t}t} \\ L_{t\bar{t}} & L_{tt} \end{bmatrix},$$

and branch relations are defined by:

$$p_L = p_L(t, f_L) = \begin{bmatrix} p_{\bar{t}}(t, f_{\bar{t}}, f_t) \\ p_t(t, f_{\bar{t}}, f_t) \end{bmatrix}.$$

In terms of mixed variables:

$$f_{\bar{t}} = f_{\bar{t}}(t, p_{\bar{t}}, f_t),$$

$$p_t = p_t(t, p_{\bar{t}}, f_t);$$

the hybrid incremental inductance matrix is:

$$\frac{\partial (f_{\bar{t}}, p_t)}{\partial (p_{\bar{t}}, f_t)} = \underline{M}(t, p_{\bar{t}}, f_t) \triangleq \begin{bmatrix} M_{\bar{t}\bar{t}} & M_{\bar{t}t} \\ M_{t\bar{t}} & M_{tt} \end{bmatrix}.$$

The inverse incremental inductance matrix is given by:

$$\frac{\partial f_L}{\partial p_L} = \underline{L}^{-1} = \underline{\Gamma}(t, p_L) \triangleq \begin{bmatrix} \Gamma_{\bar{t}\bar{t}} & \Gamma_{\bar{t}t} \\ \Gamma_{t\bar{t}} & \Gamma_{tt} \end{bmatrix}.$$

2.6 Topological Constraints on Branch Variables

2.6.1 Kirchoff's Current Law (KCL): The sum of flows in branches incident with a node is zero;

$$\sum \underline{i}(t) = 0.$$

For a network, the sum of all branch currents belonging to a cut-set is zero. The number of independent Kirchoff current equations equals the number of fundamental cut-sets of the network, $(n - 1)$. For the network, a generalized form of KCL can be written using the fundamental cut-set matrix \underline{Q}_F (Chen, 1976)

$$\underline{Q}_F \cdot \underline{i}(t) = 0.$$

2.6.2 Kirchoff's Voltage Law (KVL): The sum of branch efforts around a loop equals zero;

$$\sum \underline{e}(t) = 0.$$

The number of independent KVL equations characterizing a network equals the number of fundamental loops, $(b - n + 1)$, for a connected network. For a network, generalized KVL equations may be written in matrix form using the fundamental loop matrix \underline{B}_F (Chen, 1976)

$$\underline{B}_F \cdot \underline{e}(t) = 0.$$

2.6.3 Tellegen's Theorem: The cut space of KCL and loop space of KVL are orthogonal. The general orthogonality relation for a network is given by Tellegen's Theorem in any of its equivalent forms (Penfield et al., 1970). The sum of inner products of effort and flow vectors which satisfy Kirchoff's Laws gives the power flowing

through a network at time t :

$$\sum e_1(t) \cdot f_1(t) = 0.$$

If the network has ports, i.e., if the network is an open system, then the power at the port is distributed over the network in a small time interval (instantaneously in lumped electrical networks):

$$\sum_p e_p(\Delta t) \cdot f_p(\Delta t) = \sum_i e_i(\Delta t) \cdot f_i(\Delta t),$$

where the index p enumerates the port variables and index i , the internal system variables.

In the most general form of Tellegen's Theorem, an operator Λ' operates on branch efforts around a loop in a way that obeys KVL, and another operator Λ'' transforms flows incident on a node in a way that obeys KCL (Penfield et al., 1970). The equation for an open system then becomes:

$$\sum_p \Lambda' e_p(\Delta t) \cdot \Lambda'' f_p(\Delta t) = \sum_i \Lambda' e_i(\Delta t) \cdot \Lambda'' f_i(\Delta t).$$

A large number of operators may behave within these constraints as Kirchoff operators. Differentiation in time and integration in time are examples.

Given Tellegen's Theorem, one can derive Kirchoff's Laws (Penfield et al., 1970).

2.7 State Space Analysis of Networks

This section is drawn from presentations of Kuh and Rohrer (1965), Chua and Rohrer (1965), Stern (1964), Chua (1969), Chen (1976), Zadeh and Desoer (1963), Bryant (1959), Tow (1968), Purslow and Spence

(1967) and Brayton and Moser (1964).

2.7.1 A dynamical system is a time-varying system whose input-output relations depend on position as well as velocity (flow) and acceleration.

2.7.2 The state of a dynamical system parametrizes the relationship between the input and output vectors of the system. Knowledge of the input at $t > t_0$ and the value of system parameters at $t = t_0$ determines the output uniquely, independently of any inputs to or outputs from the system prior to time t_0 . For a one-port the state of the system is represented by a constitutive relation.

2.7.3 State variables $x(t)$ are the minimal complete set of dynamical variables which are sufficient to define the behavior of the system given inputs and the state at t_0 .

2.7.4 State space is the vector space spanned by the set of all state variables.

2.7.5 Trajectories in state space: the functional dependency of the state variables upon t , t_0 and input(s), $u(t)$.

2.7.6 The state space analysis of a dynamical system should satisfy the following conditions:

Condition 1. A real, unique output $y(t)$ exists for all $t > t_0$, given the state $x_0(t_0)$ and a real input $u(t)$.

Condition 2. A unique trajectory exists for all $t > t_0$ given $x_0(t_0)$ and a real input for all $t \geq t_0$.

Condition 3. Trajectories satisfy transition properties:

$$x_0(t) + u(t_0) \Rightarrow x(t),$$

$$x_0(t) + u(t_0) \Rightarrow x_1(t) \Rightarrow x(t).$$

Condition 4. Trajectories do not depend on inputs $u(t)$, for $(t) > t$. (Causality condition: An input cannot cause a prior effect.)

2.7.7 If the dynamical system under consideration is represented as an electrical equivalent circuit, a well-established method called the state variable approach exists for analyzing the network in the time-domain. It is based on: a) the selection of the minimal number of dynamically independent state variables using a type of spanning tree called a normal tree; b) casting branch constitutive equations of the normal tree in the normal form using KVL and KCL, that is, a system of first-order differential equations; c) elimination of dependent (non-state) variables by appropriate algebraic substitutions where necessary to derive a set of state equations. d) The resulting set of equations can be written as a product of the \underline{A} matrix and \underline{x}_1 and incorporated into the dynamical system equations:

$$\dot{\underline{x}} = \underline{A} \underline{x}_1 + \underline{B} \underline{u}_1 ;$$

$$\underline{y} = \underline{C} \underline{x}_e + \underline{D} \underline{u}_a ,$$

where \underline{x}_1 is the vector of state variables,

\underline{A} is an adjacency matrix $\underline{A} = [\underline{Q}_f^T, \underline{B}_f]$, derived from \underline{Q}_f and

\underline{B}_f matrices for normal trees and co-trees.

\underline{u}_1 is the vector of input variables

\underline{B} is the input branch matrix

\underline{u}_a is the input vector from active element sources within the network.

\underline{D} is the matrix of active branches

\underline{x}_e is the vector of output branch variables

\underline{C} is the output branch matrix.

2.7.8 Selection of a normal tree: A normal tree of the network T_N is a spanning tree that contains all the independent effort source branches, the maximum number of capacitive branches, the minimum number of inductive branches, and none of the independent flow source branches.

Its complement, the normal co-tree $T_{\bar{N}}$, contains all the independent flow source branches, the maximum number of inductive branches, the minimum number of capacitive branches, and none of the independent effort source branches.

A normal tree of a network is chosen according to a procedure given by Bryant (1959):

1. Form a capacitive subgraph or forest of a network by removing all inductive and resistive branches.

2. Form an inductive subgraph by short-circuiting all resistive and capacitive branches of the network. Choose any spanning tree of this graph.

3. Form the normal tree by the following procedure:

a) Choose any capacitive subgraph or forest including independent effort sources.

b) If the capacitive subgraph is not connected, add resistive branches until a spanning tree is formed.

c) If step b) is not sufficient to form a connected spanning tree, add a minimum number of inductive branches to form a spanning tree.

4. The normal tree may not be unique. An RLC network may have more than one normal tree.

5. Form a normal co-tree by a similar procedure:

- a) Choose any inductive subgraph including independent flow sources.
- b) If the inductive subgraph is not connected, add resistor branches to form a spanning tree.
- c) If step b) is not sufficient to form a spanning tree, add a minimum number of capacitive branches to form a spanning tree.

2.7.9 Selection of a resistive subnetwork: A resistive subgraph or forest is formed by the following procedure:

- a) Replace all capacitive branches and effort sources by short circuits.
- b) Replace inductive branches and flow sources by open circuits.
- c) Replace by open circuits all resistive branches which do not form circuits with at least one other resistive branch in the subgraph formed by steps a) and b) and remove any isolated nodes.

The resistive subnetwork may not contain all resistive branches. Excluded are resistances in parallel with a capacitance or in series with an inductance, as well as those resistances which do not form closed loops with others.

2.7.10 Selection of a set of state variables: Assign an effort and flow variable to each branch in the network. These are partitioned with respect to the normal tree and co-tree. (See Table 1)

To be considered a complete set, network variables must be chosen independently without violating Kirchoff's Laws, and determine at least one of two branch variables for each branch of the network. The voltages across normal tree capacitors and currents through co-tree inductors form a complete set of variables for a network providing

Table 1.

State Variables Chosen by Normal-Tree Method

Variables Assigned		Notation of Branches of T_N and chords of $T_{\bar{N}}$
effort variables	flow variables	
$e_{c\bar{t}}$	$q_{c\bar{t}}$	$c\bar{t}$ capacitive chords of $T_{\bar{N}}$
$e_{r\bar{t}}$	$f_{r\bar{t}}$	$r\bar{t}$ resistive chords of $T_{\bar{N}}$
$p_{l\bar{t}}$	$f_{l\bar{t}}$	$l\bar{t}$ inductive chords of $T_{\bar{N}}$
e_{ct}	q_{ct}	ct capacitive branches of T_N
e_{rt}	f_{rt}	rt resistive branches of T_N
p_{lt}	f_{lt}	lt inductive branches of T_N
e_s	f_s	independent effort and flow sources

the network has no all-capacitor loops nor any all-inductor cut-sets.

An alternative set of complete variables is the capacitor charges and inductor flux linkages (preferred for non-linear networks, so that no integrals appear in the state equations).

If a circuit of capacitors exists in a network, the chord variables are functions of the tree branch variables by KVL. A parallel statement can be made for inductor cut-sets with respect to KCL.

2.7.11 Order of complexity (degrees of freedom) is defined for a network as the number of capacitor and inductor branches less the number of capacitor loops and inductor cut-sets:

$$\sigma = b_{lc} - n_C - n_L,$$

where

b_{lc} = total number of energy storage elements in the network;

n_C = total number of fundamental loops containing only capacitor branches or capacitors and voltage sources;

n_L = total number of fundamental cut-sets containing only inductor branches or inductors and current sources.

The order of complexity for RLC networks, including networks with active branches, is equal to (1) the number of non-zero natural frequencies for a RLC network; (2) the number of arbitrary integration constants for a complete solution to normal form equations, equivalent to the number of initial conditions which must be specified (in lieu of past history of network behavior) to solve the network equations; (3) the number of state equations; (4) the number of

eigenvalues for the network (characteristic equations for the A matrix).

For active networks containing controlled source branches, an upper bound on the order of complexity can be determined if a passive normal tree (a tree composed only of linear resistors, inductors and capacitors) can be found which maximizes the difference between the number of capacitors in the tree and the number of inductors in the co-tree. It is $\sigma = \sigma_{\max} = b_{ct} + b_{lt}$. If a passive normal tree can be found, the network has a unique solution. (For proofs, and the more mathematical formulation using the H matrix, impedances and admittances rather than subnetworks, see the summary of Chen (1976) or Purslow and Spence (1967) and Tow (1968).)

2.7.12 Normal form Kirchoff's Laws: Once the normal tree and co-tree for a network are specified, and variables are assigned to branches, the matrix forms of Kirchoff Laws can be written in terms of normal tree and co-tree branches.

The normal form fundamental loop matrix is:

$$\underline{B}_f(N) = \left[\begin{array}{ccc|ccc} \underline{I}_{ct} & & & \underline{F}_{ct,t} & 0 & 0 \\ & \underline{I}_{rt} & & \underline{F}_{rt,ct} & \underline{F}_{rt,t} & 0 \\ 0 & & \underline{I}_{lt} & \underline{F}_{lt,ct} & \underline{F}_{lt,rt} & \underline{F}_{lt,t} \end{array} \right];$$

and the normal form cut-set matrix is:

$$\underline{Q}_f(N) = \left[\begin{array}{ccc|cc} -\underline{F}_{ct,t}^T & -\underline{F}_{ct,rt}^T & -\underline{F}_{ct,lt}^T & \underline{I}_{ct} & 0 \\ 0 & -\underline{F}_{rt,t}^T & -\underline{F}_{rt,lt}^T & 0 & \underline{I}_{rt} \\ 0 & 0 & -\underline{F}_{lt,t}^T & 0 & \underline{I}_{lt} \end{array} \right]$$

Kirchoff's Laws are written for a closed network in terms of normal form branch variables as:

$$\underline{B}_f(N) \cdot \begin{bmatrix} e_{ct} \\ e_{rt} \\ e_{lt} \\ e_{ct} \\ e_{rt} \\ e_{lt} \end{bmatrix} = 0; \quad \underline{Q}_f(N) \cdot \begin{bmatrix} f_{ct} \\ f_{rt} \\ f_{lt} \\ f_{ct} \\ f_{rt} \\ f_{lt} \end{bmatrix} = 0.$$

KVL equations with respect to the normal form fundamental loop matrix are:

$$e_{ct} + \underline{F}_{ct,\bar{t}} \cdot e_{ct} = 0;$$

$$e_{rt} + \underline{F}_{rt,ct} \cdot e_{ct} + \underline{F}_{rt,t} \cdot e_{rt} = 0;$$

$$e_{lt} + \underline{F}_{lt,ct} \cdot e_{ct} + \underline{F}_{lt,rt} \cdot e_{rt} + \underline{F}_{lt,\bar{t}} \cdot e_{lt} = 0.$$

KCL equations with respect to the normal form cut matrix are:

$$f_{ct} - \underline{F}_{ct,\bar{t}}^T \cdot f_{ct} - \underline{F}_{ct,rt}^T \cdot f_{rt} - \underline{F}_{ct,lt}^T \cdot f_{lt} = 0;$$

$$f_{rt} - \underline{F}_{ct,rt}^T \cdot f_{ct} - \underline{F}_{rt,lt}^T \cdot f_{lt} = 0;$$

$$f_{lt} - \underline{F}_{lt,\bar{t}}^T \cdot f_{lt} = 0.$$

2.8 Computer Methods for Analyzing Electrical Circuits.

The electronic circuit simulation program Spice 2 (Dowell et al., 1976) is used to model equivalent circuits. The types of analysis possible with this simulator are AC, DC, noise, distortion, sensitivity and non-linear time domain. Versions of Spice are available for most common main-frame and mini-computer systems from the Berkeley

Electronic Research Laboratory where the Spice program was developed. Non-linear time domain transient analysis was used to model the Brusselator system (section 4). This option determines the time domain response of the circuit with respect to specified branch elements over a specified time interval. The initial state of the system, time zero, is determined by a preliminary dc. operating point analysis. Over the time interval specified for analysis, divided into specified time points, Spice determines the steady state values for specified branches as a function of all source inputs for each time point. For example, for the time interval of 10 ms divided into ten time points, Spice will solve the network equations for ten sequential steady state values for a specified branch output and present the results as either a plot or printed table. See Appendix 1 for sample output. The state equations of the simulated network are solved using trapezoidal integration methods. Details of bench marking experiments, comparison with other integration methods, discussion of error truncation, time step control, etc., can be found in Nagel (1975).

Spice allows the option of using the Gear integration method for "stiff" equation systems which has also been used in computer simulations of chemical systems (Edelson, 1981). Benchmarking experiments with Spice comparing trapezoidal and Gear methods indicate that for circuit simulations the trapezoidal method gives results of comparable accuracy with briefer computation times (Nagel, 1975). A review of new third-generation circuit simulators can be found in Hachtel and Sangiovanni-Vincentelli (1981).

3. Network Thermodynamics

3.1 Introduction

Network thermodynamics is the study of irreversible thermodynamic systems by the design and analysis of electrical equivalent circuits. In essence the methods of network thermodynamics rest on the substitution of the energy storage and dissipation of an electrical circuit with given boundary conditions and initial state for that characterizing the thermodynamic system being modelled.

An electrical circuit is considered to be an equivalent of another system, either electrical or other physical domain(s), if the response of the equivalent to source inputs is similar in form to the modelled system. Electrical analogue circuits are equivalent circuits with the more stringent requirement that there be not only a correspondence between excitation and response, but also a proportional geometric correspondence between elements in the model system and the system being modelled (Karplus, 1958). The motivation for the construction of either type of circuit is the physical insight into the response of the modelled system provided by the circuit. Equivalence can be partitioned into dimensional, dynamical, mathematical and topological similitude which will be considered in turn below.

Methods of constructing electrical circuit analogues of many large-scale dynamical systems were developed by Kron (1944, 1963) and extended to thermodynamic systems by Peusner (1970), Oster, Perelson and associates (Oster et al., 1971, 1973; Oster and Auslander, 1971; Oster and Desoer, 1971; Oster, 1975; Oster and Perel-

son, 1974; Perelson and Oster, 1975). More recently methods for modelling dynamical systems using bond graphs were surveyed in Karnopp (1977).

The Oster and Perelson (1974) and Perelson and Oster (1975) papers are concerned with developing an abstract analysis of chemical reaction circuits based on algebraic topology. With collaboration of A. Katchalsky a series of schematics using bond graph notation (Paynter, 1961; Karnopp and Rosenberg, 1974) were developed to demonstrate how the method might be used to analyze enzyme systems and membrane transport systems of special interest to biologists and biophysicists (Oster et al., 1971; 1973). The second paper also provides a summary of electrical circuit concepts, and an extensive background bibliography. For a more recent survey, see Paterson (1980). Other examples of uses of network thermodynamics can be found in Schnackenberg (1981). An extension to probabilistic networks is discussed in Schnackenberg (1976). Finally, network thermodynamic models of membrane transport have been used by Miku-
lecky and associates (1977a, b; Wyatt et al., 1980).

Two methods of representing thermodynamic networks are available: the bond graph method with the simulation language N-port (Karnopp and Rosenberg, 1974), and equivalent circuits with a circuit simulation language, e.g., Spice (Dowell et al., 1976). Spice is presently widely used in design of electronic circuits. "Third generation" circuit simulators are even more versatile (Hachtell and Sangiovanni-Vincentelli, 1981). In contrast, N-port is not widely available and handles only linear models. The notational convenience

of bond graphs is not sufficient to outweigh the computational advantages and availability of Spice and its sequels. For this reason the formalism of electric circuits is used here exclusively.

3.2 Thermodynamic Variables and Network Equivalents

Conjugate pairs of thermodynamic variables are given by the Gibbs equation:

$$dU = TdS - pdV + \gamma dq + \sum_i \mu_i dn_i + \sum_n A \cdot J^n + \dots$$

Thermodynamic variables are cast in a form suitable for electrical equivalent circuits by the formulation of Brønsted (Lamer et al., 1949; Oster et al., 1973) which expresses conjugate pairs as the product of the difference in potential values (intensive variables which do not depend upon the size of the system) between two volumes (regions) of a system and the "quantities" or extensive variables (values of which depend on the size of the system as a whole). This product defines a "work function" with the general form

$$A = (e_1 - e_2)f,$$

which is dimensionally analogous to power in an electrical network.

Potential differences between volumes are considered to motivate flows. By taking conjugate variable pairs as products of potential differences and flows, they are expressed in the same form as across and through variables, the product of which gives energy flow or power associated with a branch of an electrical network. Across variables imply two measurements to determine potential between a branch in the network and some reference value (ground). Through

variables imply one-point measurement of flow through a branch, e.g., as measured by an ammeter. All thermodynamic intensive variables (T, p, \bar{V}, μ, A) will be taken to be across variables for purposes of constructing equivalent circuits.

The conversion of thermodynamic chemical variables to electrical network variables involves the substitution of charge for mass in the dimensional analysis, i.e., all dimensions are translated from length-mass-time (temperature) to length-charge-time (temperature). An enumeration of variables of physical domains, electrical network variables, dimensions and SI units is given in Table 2.

3.3 Dynamical Similitude

State variables of dynamical systems are functions of both space and time. Macroscopic non-equilibrium thermodynamic systems are described either by treating state variables as continuous functions of space and time, or as functions of single points in space over time described by "local" equations (DeGroot and Mazur, 1962). Equivalent circuits represent distributed networks with state variables as functions of space and time by "lumped" approximations with state variables as functions of time, assuming the spatial dimensions to contribute negligibly to the values of the state variables. This is accomplished by partitioning the distributed system into lumped subcircuit approximations with the reticulation of the lumps depending upon the accuracy required for the solution. Dynamical similitude between the thermodynamic system and equivalent circuit is based upon representing the local equations as lumped equivalents.

TABLE 2

Variables, SI Units and Dimensions

m(meter)--l(length) q(coulomb)--q(charge)

kg(kilogram)--m(mass)

s(second)--t(time)

T(thermodynamic temperature)

Generalized Variables (referring to no specific physical domain)

e(effort)

f(flow)

p(momentum)

q(displacement)

Equivalent Circuit Variables

e: v(voltage), V(volt), J(joule) C^{-1} , $l^2 m t^{-2} q^{-1}$ f: i(current), A(ampere), $t^{-1} q$ p: λ (magnetic flux), W(weber), $l^2 m t^{-1} q^{-1}$

q: q(charge), C(coulomb)=As, q

Derived Circuit Variables

P(power), e.f, W(watt), $l^2 m t^{-3}$ E(energy), f.p; e.q, J(joule), $l^2 m t^{-2}$ C(capacitance), q/e, F(farad)= CV^{-1} , $l^{-2} m^{-1} t^2 q^2$ L(inductance), p/f, H(henry), $l^2 m q^{-2}$ R(resistance), e/f, Ω (ohm), $l^2 m t^{-1} q^{-2}$ G(conductance), f/e, S or Ω^{-1} (siemens or mho)*, $l^{-2} m^{-1} t q^2$

*Obsolete, but used in Spice printout.

Chemical Reaction Variables

- e: A(affinity), J mol⁻¹(moles)
- f: J_R(reaction flow), mol s⁻¹
- q: ξ (advancement of reaction), mol
- p: ∫_t A(t).dt (not a defined variable)

Diffusion Variables

- e: μ_i(chemical potential of substance i), J mol⁻¹
- f: J_i(diffusion flow of substance i), mol s⁻¹
- q: n_i(number of moles), mol
- p: ∫_t μ_i(t) dt (not a defined variable)

Mechanical Variables

force-voltage analogy:

- e: F(force), N(Newton), J m⁻¹
- f: v(velocity) m s⁻¹
- q: q(displacement), m
- p: p(momentum), N s

force-current analogy:

- e: v(velocity)
- f: F(force)
- q: p(momentum)
- p: q(displacement)

Thermodynamic Variables

- e: T(temperature), K(degrees Kelvin)
- f: S(entropy flow), J K⁻¹ s⁻¹
- q: S(entropy), J K⁻¹
- p: not a defined variable

3.4 Mathematical and Topological Similitude

Translation of thermodynamic system equations into state equations describing an equivalent circuit requires four steps: interpretation of phenomenological equations; translation of field vectors to topological representation; conversion of conservation equations to network state equations; and conversion of entropy balance to an expression for power dissipation in a network. The thermodynamic relationships are taken from DeGroot and Mazur (1962).

The general expression for a thermodynamic phenomenological equation parametrizing the linear relation between flow J_i and the conjugate efforts X_k where all J_i 's and X_k 's are linearly independent is

$$J_i = \sum_k \mathcal{L}_{ik} X_k,$$

or the inverse for an effort and its conjugate flows:

$$X_k = \sum_i \mathcal{L}_{ik}^{-1} J_i, \quad (3.1)$$

where \mathcal{L} 's are the phenomenological coefficients. If several physical domains are involved and the system is near-to-equilibrium, coupling may occur between efforts and flows represented by off-diagonal entries in the parameter matrix (assuming an isotropic or one-dimensional system). In the linear range the parameter matrix is symmetric; the coefficients obey the Onsager reciprocal relations (Onsager, 1931a,b).

The electric circuit equivalents are the lumped circuit constitutive equations for linear branch elements. If the circuit is partitioned into a linear resistive subnetwork connected to inductor and/or capacitor ports and sources (see Chua, 1969), the impedance matrix for the resistive subnetwork has the form of eq. (3.1) where the \mathcal{L}^{-1} -coefficients are resistances. Meixner (1963) has demonstrated that the applicability of Onsager-Casimir reciprocal relations to a lumped linear electrical circuit is a consequence of the symmetry of the resistance submatrix. Any non-linear RLC circuit can be partitioned into include a symmetric resistance submatrix. (For a discussion of the case of 2-ports, see Casimir, 1963)

Thermodynamic systems modelled using equivalent circuits are not restricted to being isotropic or one-dimensional. Three dimensional field effects are represented by topological analogies to the curl and divergence vectors of the field equations (Cartesian coordinates). The procedure for topological representation of both physical domains and field effects depends to some extent upon the problems considered, but the following general comments can serve as a guide.

First, the thermodynamic system can be partitioned into basic topological units—volume elements. Within the volume element the following conditions are assumed: 1) the volume element is isothermal; 2) mass flow is absent within the element; 3) surface effects are absent. The volume element is chosen to be sufficiently small

so that events within its boundaries are functions of time only, i.e., it is a "lumped" subsystem.

Field effects then become exchanges across the boundaries of the volume elements. The analogies which can be drawn between topological laws of electric circuits, algebraic topology and vector calculus have been discussed in detail by Branin (1965). The total thermodynamic system is represented by the conservation equations as a combination of the events within and across the boundaries of the volume elements which can be considered as black boxes or sources connected to distributed branches by ports.

For a given physical domain, the divergence flow through the surface of the volume element approaches a limit as the volume diminishes to a point (Gauss' Theorem). The volume can therefore be considered topologically as a node relative to the divergence flow. If more than one volume element is present in a system, the distributed flows out of a volume element are motivated by the potential differences between volumes. The curl vector in the limit represents the potential difference over the distributed subcircuits which are topologically akin to mesh branches linking volume elements (by Stokes' Theorem).

In order to be able to apply standard network analysis techniques to equivalent circuits of distributed systems, the latter must be reduced to subcomponents representing sufficiently small spaces so that the contribution of space to the values of state variables is negligible. When state variables are functions of time only, Kirchhoff's Laws apply rather than Maxwell's equations.

Next consider the construction of an equivalent circuit representing two physical domains. For two orthogonal distributed physical domains, the force variables in one are orthogonal to the force variables in the other. In the equivalent circuit, voltages represent two different physical domains. Equivalent circuits of an electromagnetic field are an example (Kron, 1944).

Electromagnetic fields are described by Maxwell's equations (in SI units):

$$\begin{aligned} \text{curl } \underline{H} &= \frac{\partial \underline{D}}{\partial t}, & \text{div } \underline{D} &= \rho, \\ \text{curl } \underline{E} &= -\frac{\partial \underline{B}}{\partial t}, & \text{div } \underline{B} &= 0. \end{aligned}$$

The constitutive relations become

$$\underline{B} = \mu \underline{H}, \quad \underline{D} = \epsilon \underline{E}, \quad \underline{i} = \kappa \underline{E},$$

where the parameters are equivalent to impedances. \underline{D} = electric displacement, \underline{B} = magnetic induction, \underline{E} = electric field strength, \underline{H} = magnetic field strength, ρ = volume density of free charge, μ = magnetic permeability, ϵ = permittivity, κ = conductivity. For a solenoidal field (lacking free electric charges) $\text{div } \underline{D} = 0$; the electromagnetic field is conservative. Otherwise charge is not conserved.

Since an electric field is orthogonal to a magnetic field, divergence of electric displacement is orthogonal to divergence of magnetic inductance. Likewise the curl vector of electric field strength is orthogonal to the curl vector of magnetic field strength. For an equivalent circuit representing an electromagnetic field, three

distinct subnetwork paths can be identified (Kron, 1944):

(1) A mesh network—collection of closed meshes represented by electrical mesh equations ($\text{curl } \underline{E}$) and magnetic mesh equations ($\text{div } \underline{B}$).

(2) A junction (cut set) network—a collection of open meshes represented by electrical node equations ($\text{curl } \underline{H}$) and dielectric node equations ($\text{div } \underline{D}$).

(3) An orthogonal network—a collection of both open and closed meshes.

Alternatively, one may partition the complete electromagnetic equivalent circuit into an electrical network ($\text{curl } \underline{E}$, mesh equations; $\text{curl } \underline{H}$, node equations), a magnetic network which defines the path of magnetic flux lines ($\text{div } \underline{B}$, mesh equations) and dielectric network which defines the path of electrostatic flux lines ($\text{div } \underline{D}$, node equations).

Variables are also partitioned into electrical, magnetic and dielectric variables. Kron enumerates three types of currents, three types of potential differences, magnetic flux lines, electrostatic flux lines and capacitor charges as distinct variables associated with electromagnetic equivalent circuit branch elements. As is generally the case, their synthesis, or topological arrangement, is not unique.

Once the dimensional equivalences, branch constitutive relations and topological equivalences have been established, and the equivalent circuit model of the thermodynamic system constructed accordingly, the conservation equations and entropy balance for the system can be derived from the network topology.

The conservation equations for a lumped network are KVL, $\sum e(t)=0$, the efforts or potentials around a closed loop sum to zero; KCL, $\sum i(t)=0$, the sum of flows in branches incident with a node is zero. If one substitutes for effort the first order time derivative of momentum, KVL expresses the conservation of momentum around a closed path. Likewise, if the node is taken to be an arbitrary volume, the expression for KCL is equivalent to the conservation of mass with respect to the nodes.

Conservation of energy for a network (linear or non-linear lumped) is expressed by Tellegen's Theorem (Penfield et al., 1970), which can be stated in its simplest form: The sum of inner products of orthogonal effort and flow vectors which satisfy Kirchoff Laws gives the power flowing through a lumped, closed network at time t :

$$\sum e(t) \cdot f(t) = 0.$$

If the network is an open system, Tellegen's Theorem can be written:

$$\sum_p e_p(\Delta t) \cdot f_p(\Delta t) = \sum_i e_i(\Delta t) \cdot f_i(\Delta t),$$

where the index p enumerates the port variables and index i the internal system variables. The power (energy flow) applied at the ports equals that flowing within a lumped network over a given time interval.

For an equivalent circuit representing n orthogonal physical domains, open to flows of energy from surroundings, the conservation of energy can be written using Tellegen's Theorem as a direct sum of the internal energy flows for each physical domain subcircuit:

$$\sum_p e_p(\Delta t) \cdot f_p(\Delta t) = \sum_{i(1)} e_{i(1)}(\Delta t) \cdot f_{i(1)}(\Delta t) +$$

$$+ \left(\sum_{i(2)} e_{i(2)} (\Delta t) \cdot f_{i(2)} (\Delta t) \right) \\ + \dots + \left(\sum_{i(n)} e_{i(n)} (\Delta t) \cdot f_{i(n)} (\Delta t) \right).$$

Taking the lumped circuit to represent a volume element this expression is the equivalent of the expression for conservation of energy for an isothermal volume element given by DeGroot and Mazur (1962):

$$\left(\frac{\partial \rho_e}{\partial t} \right)_V = - \operatorname{div} \underline{J}_e.$$

The change in energy density ρ_e within an arbitrary volume equal to the energy flow \underline{J}_e through the boundary is a function of potential, kinetic and internal energy of the volume element.

For a distributed network, Maxwell's equations apply rather than Kirchoff's Laws, and the conservation of energy is given by the Poynting Theorem. An expression for Tellegen's Theorem using Kirchoff Operators derived from the Poynting Theorem is given by Penfield et al. (1970).

Tellegen's Theorem can also be used to derive a variational expression for the dissipation of power due to resistances within a (non-linear) circuit relative to the power applied at the ports (Penfield et al., 1970). Given a function $G = \int_0^1 v \, di$ with dimensions of power, for a linear network

$$G(i_p^0) = \sum_{\alpha} G_{\alpha}(i_{\alpha}^0)$$

where i_p^0 are the currents at the ports computed from the network constitutive equations. If there are variations in current flow due to heat effects, viewed from the ports, the currents are i_p , which may vary from i_p^0 . From Millar's work (1951) one can prove that

$$G(i_p) - G(i_p^0) = \sum_{\alpha} G_{\alpha}(i_{\alpha}) - G_{\alpha}(i_{\alpha}^0),$$

where the superscript zero indicates the computed current values, the subscript p indicates values at the ports, and α , the internal branch values. Considering only positive resistors, one finds that

$$v_{\alpha}^0 (i_{\alpha} - i_{\alpha}^0) \leq G_{\alpha} i_{\alpha} - G_{\alpha}(i_{\alpha}^0)$$

for a given resistive branch. Summing over the branches and using Tellegen's Theorem gives

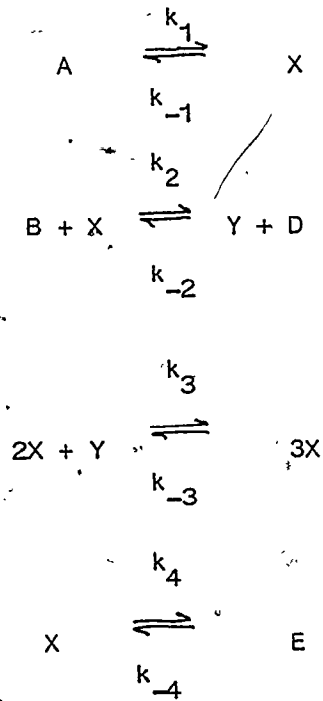
$$\sum_p v_p^0 (i_p - i_p^0) \leq \sum_{\alpha} G_{\alpha}(i_{\alpha}) - \sum_{\alpha} G_{\alpha}(i_{\alpha}^0).$$

If currents i_{α} are compatible with KCL and the boundary conditions of the network, the left hand side of the inequality equals zero; content due to the variation in the current cannot be less than that computed from correct currents. Increases in current flow accompany dissipation due to heat effects. Therefore this expression could be used to derive an expression for entropy balance.

4. Equivalent Circuit Model of the Brusselator Reaction-Diffusion System

4.1 Introduction

The chemical reaction-diffusion system known as "Brusselator", proposed and studied by I. Prigogine and associates in Brussels, is represented by the sequence of reactions:



If the forward rate constants, k 's, are all set to +1 and the reverse k 's set to -1, rate equations for the reversible reactions written in terms of the intermediates X and Y are (Glansdorff and Prigogine, 1970):

$$\frac{dX}{dt} = (A + X^2 Y - BX - X) + (-YD - E + X - X^3)$$

$$\frac{dY}{dt} = (BX - X^2 Y) + (-X^3 + YD)$$

Interest in the Brusselator as a model derives from the fact that it is the simplest reaction-diffusion system with two intermediate variables capable of limit cycle behavior (Tyson and Light, 1973). The behavior is a consequence of the non-linear trimolecular step when the system is sufficiently far from equilibrium—a condition determined by the initial state, appropriate boundary conditions, reaction affinities and diffusion coefficients.

The trimolecular step is necessary; a system with two intermediate variables, but only uni- or bimolecular reaction steps cannot exhibit limit cycle behavior. This has been stated as a theorem and formally proven by Nicolis and Prigogine (1977). Because the trimolecular step would proceed very slowly in an actual reaction, the model is considered to be realistic only in the sense that it does not violate any of the laws of physics or chemistry (Tyson and Light, 1973). If the trimolecular step is replaced with a sequence of enzyme reactions with the same overall order, the limit cycle behavior is retained, but the model is a more realistic example of biochemical reactions (Tyson, 1973).

The simplicity of the Brusselator model also makes it a suitable example with which to explore the types of analysis for which equivalent circuit models of reaction-diffusion systems are particularly useful. Using the Spice circuit simulation language (Dowell et al., 1976), circuit response in the time domain may be analyzed using the dc transient analysis option. This is applied below to analysis of zero-input reaction circuit models with specified initial capacitor voltages, and models of distributed reaction-diffusion equivalent cir-

cuits with pulsed current sources. Solutions to problems met in constructing these models of the Brusselator can be applied to morphogenetic systems of more biological interest, particularly those where an enzyme transport system operates simultaneously in several locations within a cell or organ.

Theory and numerical simulations of the Brusselator model are presented in a series of papers published by Prigogine and associates (Prigogine and Nicolis, 1967; Lefever et al., 1967; Prigogine and Lefever, 1968; Edelstein, 1970; Herschkowitz-Kaufman and Nicolis, 1972; Herschkowitz-Kaufman, 1975; Lefever et al., 1977) as well as papers by Tyson (1973), Tyson and Light (1973), Hanusse (1972), Noyes and Field (1974) and Richter et al. (1980). Most of these are reviewed by Glansdorff and Prigogine (1971), Nicolis and Prigogine (1977), Prigogine and Lefever (1978) and Fife (1976,79). Nicolis and Prigogine (1977) in particular give a careful discussion of theory, background mathematics and numerical simulations of the model. A discussion more accessible to the non-technical reader can be found in Prigogine (1978).

The published analyses of the Brusselator fall into two categories: first, the study of thermodynamic properties of steady-state maintenance of dissipative structures and limit cycles through diffusion coupled with reactions (entropy sources); and second, the identification and description of instabilities and the conditions when these cause the transformation from an equilibrium or near-to-equilibrium homogeneous steady state to two or more non-homogeneous far-from-equilibrium steady states. Steady states can be adequately

analyzed with non-equilibrium thermodynamic methods discussed in Section 3. The equivalent circuits of the Brusselator presented below are limited to numerical simulations of steady state, macroscopic, deterministic models.

At the critical point the system becomes unstable or sensitive to small perturbations. The deterministic, macroscopic steady state descriptions are not valid because statistical assumptions implicit in these models break down. The behavior of the Brusselator around the critical point has been examined by two general methods (reviewed by Nicolis and Prigogine, 1977): stability theory including Lyapunov methods, and bifurcation theory used to examine system trajectories at the points of instability. Note that both methods can be applied to equivalent circuit models as well. (See Stern (1964) for Lyapunov methods; Andronov et al. (1966) for limit cycles in electrical circuits and van der Pol oscillators; Mees and Chua (1979) for bifurcation theory (Hopf bifurcations) applied to electrical circuits.)

4.2 Construction of Equivalent Circuit Model of the Brusselator

Rules for construction of linear, near-to-equilibrium models of chemical reactions using equivalent circuits were outlined in Perelson and Oster (1975). (Most models discussed in publications by Oster and colleagues are based on bond graphs, cf. also Paterson, 1980).

Assumptions made in constructing the Brusselator circuit model are: (1) Solvent effects are negligible and ignored. (2) Vol-

lume(s) are unit volumes. (3) Volume(s) and temperature are assumed to be constant. (4) Volume element subcircuits represent structurally homogeneous subsystems. (5) All reactions are reversible. (6) Inputs to reaction elements represent inputs of substances A and B. (7) Substances D and E are removed from the open circuit system passively through node to ground ammeters. (8) The diffusion system is one-dimensional and can be described by Fick's first law.

These are similar to assumptions made by Herschkowitz-Kaufman (1975), also discussed in Nicolis and Prigogine (1977), with exception of assumption (5). In the Herschkowitz-Kaufman model forward rate constants are set at infinity, reverse rate constants at zero, making the system irreversible and as far from equilibrium as possible. In contrast, the reaction subcircuit is initially modelled as a linear, near-to-equilibrium, zero-input system to establish the base response of the circuit. The circuit is then systematically biased to a far-from-equilibrium state. The reversibility of flows through reaction subcircuits tends to stabilize the whole system.

The equivalent circuit model also differs topologically from most of those considered by the Prigogine group. Their models begin with one homogeneous volume within which the distribution of intermediate reactant X evolves over time, given proper boundary conditions, to non-homogeneous distribution over space. The equivalent circuit model has a set number of volume subcircuits with the same initial values for reactants. The development of spatial inhomogeneities is measured over time increments as changes in potential (voltage) at fixed positions within the circuit (capacitors repre-

senting X and Y in each volume subcircuit).

As a consequence of these differences between the two model types, one can expect the circuit model to show at best qualitative similarities to results of the earlier numerical simulation models. The equivalent circuit model is a unique, but complementary, analysis in its own right.

Construction and analysis of an equivalent circuit of the Brusselator is based upon dimensional, dynamical, topological and mathematical similitude between the circuit model and the thermodynamic model.

4.3 Dimensional Equivalence

Dimensionally the Brusselator involves reaction and diffusion domains. Hydrodynamic flow is assumed to be absent. The appropriate effort and flow variables and SI units (from Table 2, Section 3) are:

Chemical Reaction:

e: affinity, A , $J \text{ mol}^{-1}$

f: reaction flow, $J_R = d\xi/dt$, mol s^{-1}

q: advancement of reaction, ξ , mol

p: $\int^t A(t) dt$ (not a defined variable)

Diffusion:

e: chemical potential of substance i , μ_i , $J \text{ mol}^{-1}$

f: diffusion flow of substance i , J_i , mol s^{-1}

q: number of moles (or concentration) of substance i , $n_i(c_i)$, mol
(mol m^{-3})

$p: \int_{x_1}^x dt$ (not a defined variable)

Equivalent Circuit Variables:

$e: v$ voltage, V, J C⁻¹

$f: i$ current, A, C s⁻¹

$q: q$ charge, C

$p: \lambda$ flux linkage, W

4.4 Topological Equivalence

The topology of a reaction-diffusion system can be resolved into the distinct subcircuits for each physical domain. The reactions can be represented by a lumped circuit because by assumption space is not a factor affecting the reaction within the volume. All variations in concentrations of reactants and products over space and time are assumed to fall in the diffusion subcircuit. Coupling between the two subcircuits is accomplished by embedding the lumped reaction subcircuits topologically as nodes connected by diffusion distributed subcircuits as branches.

4.4.1 Distributed Subcircuit.

In Spice realization the distributed subcircuit is represented as a series of lumped black box transmission line approximations characterized by an impedance and a time delay for each transmission line (Fig. 4). The paths of diffusion flow are represented topologically using transmission lines connecting the volume elements. For the one-dimensional Brusselator circuit, reaction subcircuits are connected in series with transmission lines with each line representing diffusion of X or Y. The X and Y lines form parallel subcircuits

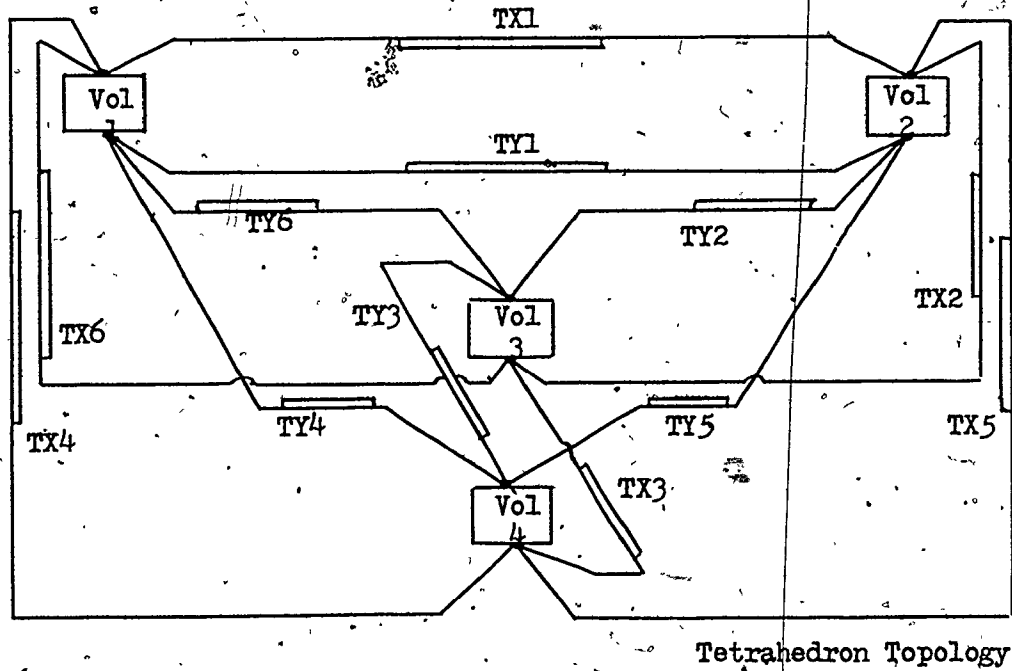
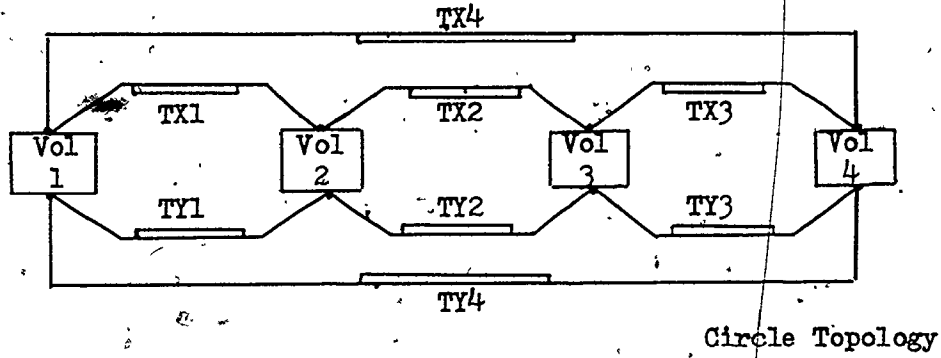
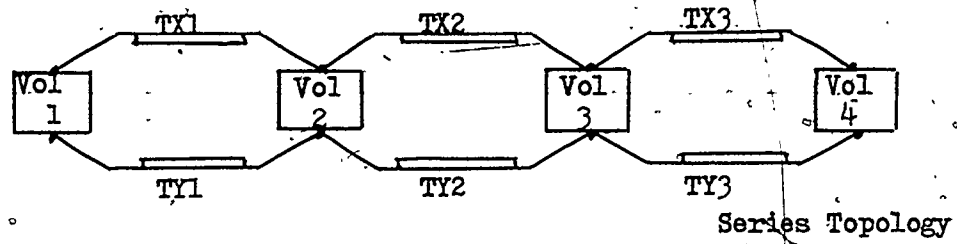


Figure 4. Distributed Reaction-Diffusion Network

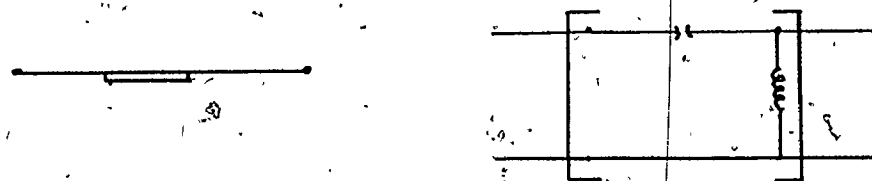
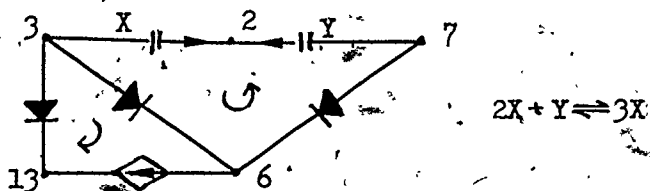
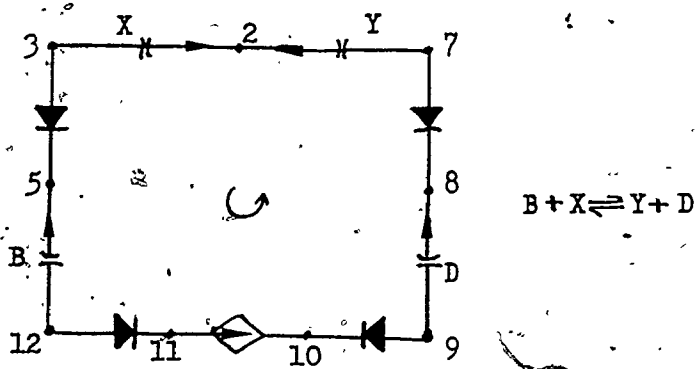
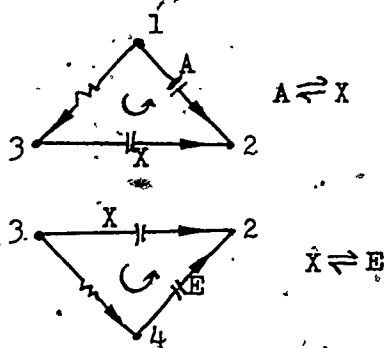


Figure 5. Spice Equivalent Circuit for Transmission Line Segment



Reaction Subcircuits:

Figure 6

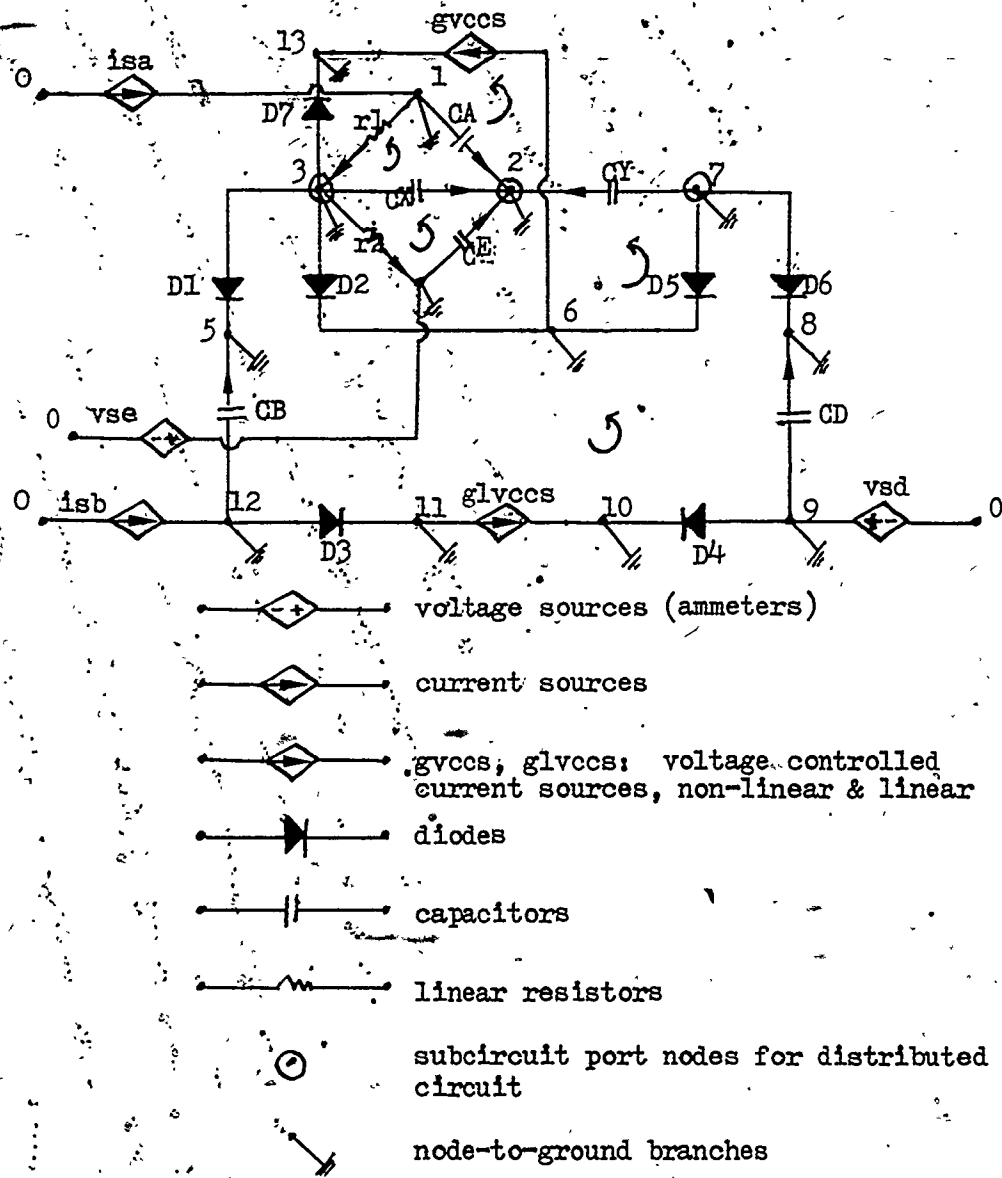
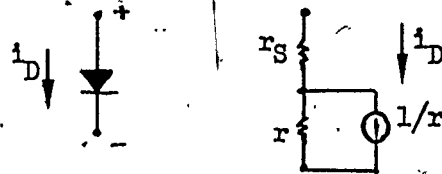


Figure 7. Spice Open Reaction Subcircuit



Diode Model Equivalent Circuit and Branch Orientation
 Figure 8

between volume element nodes. There is no coupling between the representative transmission lines. For two or more dimensional arrays the number of transmission lines and volume subcircuits must be increased. As an alternative to the Spice transmission line, one could use the elements representing the distributed subnetwork. This would be a necessity for models of non-linear diffusion, and models where coupling occurs between diffusing substances.

The transmission lines are connected to the positive nodes of the X and Y capacitor branches. Once the reaction subcircuits are embedded as nodes in the transmission line network, they become black boxes whose behavior can be measured only at ports. The X and Y capacitors serve as ports for both reaction subcircuit and transmission line black boxes.

4.4.2 Chemical Reaction Subcircuit.

Each reversible chemical reaction is represented by a loop composed of a capacitor for each substance participating as a reactant or product, transducing element(s) gating the current to stoichiometric proportions into a resistor element which serves as a dissipation element connecting the reactant domain to the product domain. The orientation of the loop is taken to be the same as that of the resistor element. In first order reactions, the reaction loop is a fundamental loop; the resistor branch—the chord which defines the orientation of the loop; and other loop elements—spanning tree branches (Penelton and Oster, 1975). This partitions elements representing reactants, products and transducers into the spanning tree sub-

space and the resistors into the cut-set subspace. The spanning tree subspace is orthogonal to the cut-set subspace. Therefore orthogonality is imposed upon the dissipation and energy storage aspects of a linear chemical reaction in the network equivalent by the topological partitioning of the circuit. In models of non-linear autocatalytic reactions with bimolecular or higher order reaction steps, this interpretation may not hold because removing the resistor branches fails to remove all loops from the circuit, for example, the circuit for $2X + Y \rightleftharpoons 3X$ where the forward orientation for the non-linear resistor (voltage controlled current source) forms a positive feedback loop.

Each reaction is coupled through one or more capacitors in common with other subreactions. In the case of the Brusselator, the capacitor representing substance X is common to each subreaction, and thus serves as a coupling element for the reaction loops.

The distinctness of reacting substances in the network is lost in the conversion of chemical variables to their electrical equivalents; the distinctions must be retained topologically. In open circuits, each substance input to or output from the circuit is represented by a port adjacent to the appropriate capacitor at the positive node. The composition of the Brusselator reaction subcircuit is diagrammed in Figures 6 and 7.

4.5 Mathematical Similitude

The relationship between chemical kinetic equations, reaction stoichiometry, free energy changes and the constitutive and circuit equations were summarized by Oster et al. (1973, see also Paterson,

1980), and this reference is the basis for portions of the following discussion. The mathematical description of the equivalent circuit differs from the usual kinetic equations in several important respects: (1) The construction of the equivalent circuit imposes an explicit topology upon the relations between reactants and products and energy dissipation. (2) The constitutive relations include both flow and effort variables. (3) Electrical circuit branch outputs are given in terms of voltages rather than currents in Spice.

4.5.1 Diffusion Subcircuit.

Take the change in moles of substance i due to diffusion in one dimension to be

$$\frac{dn_i}{dt} = -D \frac{d\mu_i^T}{dx},$$

where $d\mu_i^T/dx$ is the density gradient, D is the coefficient of diffusion (Fick's First Law). In the Brusselator equivalent circuit the terms of the above equation have the following interpretations: dn_i/dt is the current flow through capacitor i , where i is substance X or Y , due to the diffusion subcircuit, D is the admittance of the distributed subcircuit, $d\mu_i^T/dx$ is the voltage drop over the line represented by the time delay, a measure of line length. Spice gives printouts of capacitor voltages:

$$\mu_i(t) = Z\theta \frac{dx}{dn_i^T} dt,$$

where $\mu_i(t)$ is the capacitor voltage due to transmission line operation of the X or Y capacitors, $Z\theta$ is the line impedance, dn_i^T is the line charge change or capacitor current.

4:5.2 Reaction Subcircuit.

Boundary Conditions: For the equivalent circuit boundary conditions are either closed (zero-input) with no source element operating, or open with rectified current sources representing inputs of substances A or B. Spice allows specification of duration, time step and magnitude of current pulses. Passive removal of substances D and E from the system is represented by grounded voltage source ammeters. For the distributed circuit, sources operate independently to each volume element.

Stoichiometry: The topological orientation of each capacitor branch with respect to the orientation of the resistor chord of a fundamental reaction circuit determines the sign of the capacitor branch in the fundamental loop and cut-set matrices. To correspond to the signs of the stoichiometric coefficients, the reactant capacitors are oriented opposite to the resistors giving them a negative sign. Product capacitors are oriented in the same direction giving them a positive sign.

Division of a reaction circuit into capacitors and a resistor corresponds to the energy storage and energy dissipation domains. In keeping with this distinction the change from one domain to the other is mediated by transducers to hold capacitor flow to and from the dissipation element to stoichiometric proportions (rather than absolute values). In the Spice realization of the Brusselator, this function is approximated by using reversible diodes. The forward flow through the diode is controlled by the saturating current parameter; the reverse is controlled by the emission coefficient. These

parameters can be set independently. For the Brusselator model the parameters are set by adjusting diode voltages for the zero-input circuit model. The equivalent circuit for this ideal diode is diagrammed in Figure 8.

Reaction Rates, Constitutive Relations and Circuit Equations: In a closed reaction volume, the changes in moles of reactants and products are governed by the relationships:

$$\frac{dn_i}{\nu_i} = d\xi; \quad J^R = \frac{d\xi}{dt},$$

where ν_i is the stoichiometric coefficient of the i th substance, ξ is the advancement of the reaction, and J^R is the reaction flow. Distinguishing forward and reverse stoichiometric coefficients, ν_i^f and ν_i^r respectively, time rate of change of substance i is:

$$\frac{dn_i}{dt} = \nu_i J^R = -(\nu_i^f - \nu_i^r) J^R,$$

where $-\nu_i = (\nu_i^f - \nu_i^r)$. If a substance n_i participates in more than one concurrent reaction, the rate of change due to the k th reaction becomes:

$$\frac{dn_i}{dt} = - \sum_{k=1}^M \nu_{ik}^f J_k^R + \sum_{k=1}^M \nu_{ik}^r J_k^R.$$

The effort variable for chemical reactions, affinity A , is defined by the following relations:

$$A = \sum_{i=1}^N -\nu_i^f \mu_i = \sum_{i=1}^N \nu_i^r \mu_i.$$

Distinguishing forward and reverse affinities,

$$\underline{A} = \underline{A}^f - \underline{A}^r,$$

where

$$\underline{A}^f = \sum_{i=1}^N \nu_i^f \mu_i; \quad \underline{A}^r = \sum_{i=1}^N \nu_i^r \mu_i.$$

Close to equilibrium a linear relationship exists between affinity and reaction rate governed by the constitutive equation for a linear resistor:

$$J^R = 1/R \underline{A}$$

Far from equilibrium there is no general expression relating reaction rate and overall affinity. In this case the relationship between affinity and reaction rate can be derived as follows (Oster et al., 1973; Paterson, 1980).

First, the reference affinities, that is affinities of reactants and products in their standard states ($\mu_i = \mu_i^0$) are related to the equilibrium constant K_{eq} .

$$\underline{A}_0^f = \sum_{i=1}^N \nu_i^f \mu_i^0; \quad \underline{A}_0^r = \sum_{i=1}^N \nu_i^r \mu_i^0;$$

$$\underline{A}_0^f - \underline{A}_0^r = \sum_{i=1}^N \nu_i \mu_i^0 = RT \ln K_{eq}. \quad (4.1)$$

Next the relationship between J^R and K_{eq} is derived. For mass action kinetics:

$$J^R = k_f \prod_{i=1}^N c_i^{\nu_i^f} - k_r \prod_{i=1}^N c_i^{\nu_i^r}$$

where k_f is the forward rate constant, k_r is the reverse reaction rate constant. At equilibrium the net reaction rate is zero; therefore,

$$k_f/k_r = K_{eq} \quad (4.2)$$

Combining equations (4.1) and (4.2)

$$k_f \exp\left(-\frac{A_o^f}{RT}\right) = k_r \exp\left(-\frac{A_o^r}{RT}\right) \triangleq K$$

By assuming a mixture is ideal, chemical potential is $\mu_i = \mu_i^o + RT \ln c_i$ and $c_i = \exp(\mu_i - \mu_i^o)/RT$. The relationship between reaction rates and affinities is then:

$$\underline{J}^R = K \exp\left(\frac{A^f}{RT}\right) - K \exp\left(\frac{A^r}{RT}\right),$$

or equivalently

$$\underline{J}^R = v^f - v^r;$$

where $v^f = K \exp(A^f/RT)$ and $v^r = K \exp(A^r/RT)$.

When \underline{J}^R is not equal to zero, the constitutive relationship between \underline{J}^R and \underline{A} is represented by a non-linear resistor, voltage-controlled current source (VCCS) in Spice with a current gain exponent set as the sum of the stoichiometric coefficients for the reactants. Since moles or concentrations are converted to charge in the equivalent circuit, assuming mass action kinetics, the sum of reactant stoichiometric coefficients equals the sum of product coefficients. With constant parameters the proper higher order term is thus maintained for both positive and negative current through the VCCS. The consti-

tutive equation for the non-linear VCCS is:

$$\underline{G}(t, e_R) = \partial \underline{i}'_R / \partial v_R,$$

which is solved in Spice, by expansion in a power series of up to twenty terms.

Recalling the mass-charge analogy, the relation between the number of moles and chemical potential for each chemical species in terms of capacitor charge and capacitance for substance i is:

$$n_i = \sum_{j=1}^N C_{ij} \mu_j,$$

where C_{ij} is an element in the capacitance matrix, and n_i is a function of all μ_j 's. The constitutive relation for capacitor flow for substance i in terms of the potential μ_i of substance i is

$$\frac{dn_i}{dt} = C_{ii} \frac{d\mu_i}{dt}.$$

The capacitor flow for substance i , dn_i/dt as a function of all other capacitor potentials is:

$$\frac{dn_i}{dt} = \sum_{j=1}^N C_{ij} \frac{d\mu_j}{dt},$$

where C_{ij} is an off-diagonal element in the capacitance matrix. The inverse relationship expresses the potential μ_i of substance i as a function of all capacitor flows:

$$\frac{d\mu_i}{dt} = \sum_{j=1}^N S_{ij} \frac{dn_j}{dt},$$

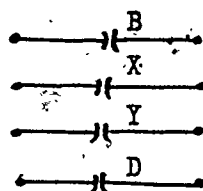
where S_{ij} is an off-diagonal element in the elastance matrix. Since each substance is represented by one capacitor, the order of complexity (eigenvalues or degrees of freedom) of the reaction sub-circuit is the same as the number of substances participating in the volume reactions, excepting solvent effects which are assumed to be absent. Assigning values to capacitors is based on the assumption that the Brusselator solution is ideal (for the equilibrium reaction sub-circuit):

$$C_i = \frac{dn_i}{d\mu_i} = \frac{n_i}{RT} = \frac{c_i V}{RT}$$

4.6 An Illustration of the Construction of an Equivalent Circuit for a Reversible Linear Reaction (close to equilibrium)

To illustrate the discussion of sections 4.4.2 and 4.5.2, consider the following reaction: $B + X \rightleftharpoons Y + D$.

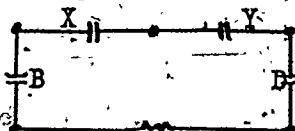
1. Substances B, X, Y and D are represented by lossless capacitors.



The constitutive relation for the chemical capacitance C_B and its electrical equivalent are:

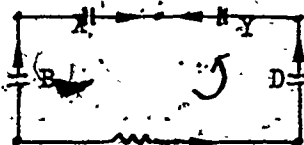
$$\frac{dn_B}{dt} = C_B \frac{d\mu_B}{dt}, \quad i = C_B \frac{dV}{dt}$$

2. Formation of Reaction Loop: The change in free energy between reactants and products is represented by a resistor chord forming a loop with the capacitors. Orientation of the loop corresponds to that of the resistor branch, i.e., corresponds to positive current flow through the resistor branch. The constitutive relations for the chemical reaction domain and electrical equivalent



are: $J_R = 1/R A$; $i = 1/R v$, where J_R is reac-

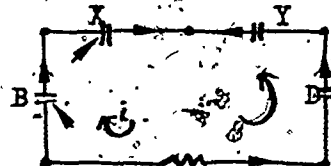
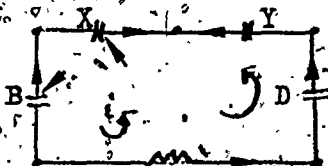
tion flow, A is affinity, R is resistance. Orientation of capacitor branches is given by the stoichiometric coefficients which are negative for reactants and positive for products. The sign of



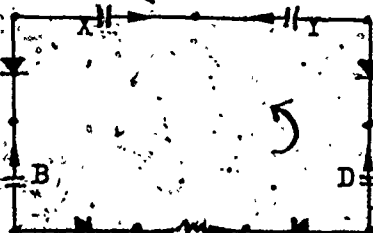
the loop branches is determined by their orientation with respect to the chord; product capacitors are given the same or-

ientation as the chord. Parameter values can be set from relations for linear reactions (Sect. 4.5.2). However, for simplicity, unit resistors were used for linear reactions.

3. The initial closed linear circuit transient current flow direction depends upon which plates of the reactant capacitors are charged. Arrows indicate capacitor plates charged at $t = 0$ (specified as initial conditions in Spice program), and i-labelled bent arrows indicate resulting initial current flow direction in the circuit.



4. Finally, to hold the flow from the capacitors of the energy storage domain to stoichiometric proportions through the resistor of the energy dissipation domain, transducers in the form of diodes are inserted at the positive nodes of each capacitor.



4.7 Results and Discussion

Plots of the transient analyses of the Brusselator circuit for the voltages of the CX capacitors as a function of time follow this section. For a sample complete Spice printout, see Appendix 1. The purpose of the sequence of programs is to demonstrate the use of Spice to model the Brusselator system in a manner which is applicable to more complicated distributed biological reaction pathways. For example, the structure of the subcircuit programs allows the comparison of isolated functions of the subcircuit with respect to branch variables of interest, and the same subcircuit in different topological contexts. Interaction and resonance effects are particularly easy to study with suitable equivalent circuits. Spangler and Snell (1967a,b) have explored the use of transfer functions in studying oscillatory enzyme reaction systems. One can directly analyze such systems in the time domain using Spice transient analysis option rather than having to turn to the use of Laplace transforms and linear frequency domain analysis. Because all thermodynamic variables are expressed in common dimensions in equivalent circuits, Spice models can be used to simulate interactions between several physical domains and kinetics of chemical reactions or the behavior of chemical reactors in process control (Edelson, 1981 and Westerberg, 1981 respectively).

The following discussion considers the sequence of equivalent circuit models of the Brusselator system. The boundary conditions for the open circuit are given by the current sources and ammeters which represent mass flow into and out of the circuit volume(s) respectively. Since Spice branch output values are given as voltages, to obtain

values for current (mass flow) or charge (mass) one must substitute voltage values in the appropriate constitutive equation (Sect. 4.5.2).

Plot 1 provides a base response for the closed reaction subcircuit (schematic diagram, Figure 8) with zero inputs. Capacitors are assigned initial voltages in stoichiometric proportions. To compare with subsequent distributed circuit responses, two types of open reaction subcircuit are analyzed: first, the system with linear reaction dissipation branches (plot 2) and secondly, the open system with non-linear resistor operating (plot 3). The comparison shows that the increased positive feedback current gain, given the same boundary conditions as previously, increases the amplitude of oscillations in the capacitor voltage.

Plots 5, 8, 9, 10, 11, and 12 for the series connected distributed circuit (series topology schematic, Figure 4) demonstrate the effects of varying the impedance and time delay parameters. For all of these circuits the sources are operating in volume 4 only imposing an asymmetry on the current flow through the distributed circuit. Plot 5 gives the circuit response when the source representing reactant B in volume 4 subcircuit is pulsed at .015s intervals for durations of .005s with a magnitude of 5 amps. The current source representing reactant A provides a constant 1 amp bias to the volume 4 subcircuit.

Plot 8 is from the same circuit in all respects, but time delays on tx lines (transmission lines representing the movement of substance X by diffusion between subvolumes) are changed from .001s to .005s. This results in longer periods in the oscillations of the voltages of the CX capacitors with a decrease in amplitude of voltage oscillation for volumes 1, 2, and 3, and an increase for volume 4.

For plots 10 and 11 the impedances are doubled for the tx and ty lines respectively. In plot 10 the period of oscillations is unaffected, but the amplitude of oscillations of voltage values for capacitors CX in volumes 1, 2, and 3 is decreased; for volume 4 the amplitude is increased. Changing the impedances of the ty lines produces little change in CX voltages.

Plot 12 is the output from the distributed circuit where both impedances and time delays are varied for tx and ty lines with sources operating in volume 4 as previously. This arrangement produces the most asymmetric circuit possible with constraints of constant parameters and the source inputs used in the previous circuits to allow comparison of response. The net effect is the stabilization of CX voltage in volume 1 over time, with the CX voltage response in volume 2 oscillating around the volume 1 values. For comparison plot 13 circuit has the same parameter settings but sources operating into each volume subcircuit. The CX capacitor responses mirror the pattern of pulses. To see effects of td and z0 settings would require that the pulse magnitudes be decreased by approximately a magnitude of 10 to values more consistent with the current transferred between volume subcircuits when only one pair of sources is operating.

If the circuit is excited by only one pulse and then allowed to relax to a steady-state, the equivalent circuit provides a way of simulating relaxation methods used to study chemical reaction systems. The series of plots #4, 6, 7, 15 and 19 demonstrate this use. Plots 6 and 7 are series topology circuits (compare with plot 5) with magnitudes of the pulse current source i_{sp} of 5 and 15 amps respectively. The stronger pulse results in a voltage value of CX in volume 3 different

from that of volumes 1 and 2; volume 4 assumes the same mean value for both circuits.

Increasing the number of diffusion pathways between volume elements, circle and tetrahedron topologies (Figure 4), respectively plots 14 and 18, increases the amplitude of voltage oscillations in the CX capacitors relative to the series topology with the parameter settings used, but do not produce any stable asymmetries in response between volume elements in the open circuit.

Construction of an equivalent circuit model of the Brusselator reaction system demonstrates the steps one can take to construct a model of an open, non-linear reaction-diffusion system. The reaction sequence is very simple relative to those found in biological systems, but of sufficient complexity to pose problems in synthesis which must be considered in constructing more complex models. As noted in section 4.2 the circuit model differs from other published simulations in a number of respects, particularly in the iteration of reaction volume elements to represent the local partitions of the spatial dimensions of the diffusion space. The stable oscillations in concentrations of X over space, a property of the Brusselator under appropriate boundary conditions noted in numerical simulation models (Nicolis and Prigogine, 1977), have been shown to occur in the circuit model in its most asymmetric form (plot 12, Figure 9) as differences in potential and magnitude of oscillations in the values of X capacitors for each volume element. The limit cycle behavior of the steady state circuit model has not yet been examined.

Figure 9

Description of Equivalent Circuits for Plots of CX Capacitor Voltages Determined by Transient Analysis Using Spice:

1. Brus 1.4 Reaction subcircuit (schematic diagram Figure 8): linear resistors, zero input, initial conditions—capacitor voltages specified for system state at $t = 0$.
2. Brus 1.4a Reaction subcircuit (schematic diagram Figure 8): linear resistors, zero state, current source isa set to constant value of 1 amp, current source isb pulsed at 1 amp.
3. Brus 1.4b Reaction subcircuit (schematic diagram Figure 8): same as Brus 1.4a except that non-linear voltage controlled current sources replace resistors r3 and r4.
4. Brus 1.4b1 Reaction subcircuit (schematic diagram Figure 8): same as Brus 1.4b, but current source isb pulsed only once.
5. Brus 1.4c Distributed reaction-diffusion circuit (series topology schematic, Figure 4): zero-state, series connection of volume sub-circuits, current sources on in volume 4 only, non-linear resistors, equal impedances and time delays, capacitor voltages CX plotted for each volume subcircuit.
6. Brus 1.4c1 Distributed reaction-diffusion circuit (series topology schematic, Figure 4): same as Brus 1.4c, but current source isb, volume 4 pulsed only once, 5 amp.
7. Brus 1.4 c2 Distributed reaction-diffusion circuit (series topology schematic, Figure 4): same as Brus 1.4c, but current source isb volume 4 pulsed only once, 15 amp.

8. Brus 1.4d Distributed reaction-diffusion circuit (series topology schematic Figure 4): same as Brus 1.4c, but time delays of tx lines changed from .001s to .005s.

9. Brus 1.4e Distributed reaction-diffusion circuit (series topology schematic Figure 4): same as Brus 1.4c, but time delays of ty lines changed from .001s to .005s.

10. Brus 1.4f Distributed reaction-diffusion circuit (series topology schematic Figure 4): same as Brus 1.4c, but impedances of tx lines doubled, i.e., resistance to diffusion of substance X is twice that to substance Y.

11. Brus 1.4g Distributed reaction-diffusion circuit (series topology schematic Figure 4): same as Brus 1.4c, impedances of ty lines doubled, i.e., resistance to diffusion of substance Y is twice that to substance X.

12. Brus 1.4h Distributed reaction-diffusion circuit (series topology schematic Figure 4): same as Brus 1.4c, but impedances, time delays for each line set to different values.

13. Brus 1.4i Distributed reaction-diffusion circuit (series topology schematic Figure 4): same as Brus 1.4h, but all volume sources operating at different pulse intervals, same magnitudes.

14. Brus 1.4j Distributed reaction-diffusion circuit (circle topology Figure 4): same as Brus 1.4i, but distributed network circle topology rather than series.

15. Brus 1.4j2 Distributed reaction-diffusion circuit (circle topology schematic Figure 4): same as Brus 1.4j, but sources in volume 4 only, 4sb pulsed once.

16. Brus 1.4l Distributed reaction-diffusion circuit (circle topology schematic Figure 4); same as Brus 1.4j, but only tx lines operating, a simulation of the situation where only substance X can diffuse.

17. Brus 1.4m Distributed reaction-diffusion circuit (series topology schematic Figure 4); same as Brus 1.4i, but one pulse for each current source isb.

18. Brus 1.4n Distributed reaction-diffusion circuit (tetrahedron topology schematic Figure 4); same as Brus 1.4i, but distributed network tetrahedron topology rather than series.

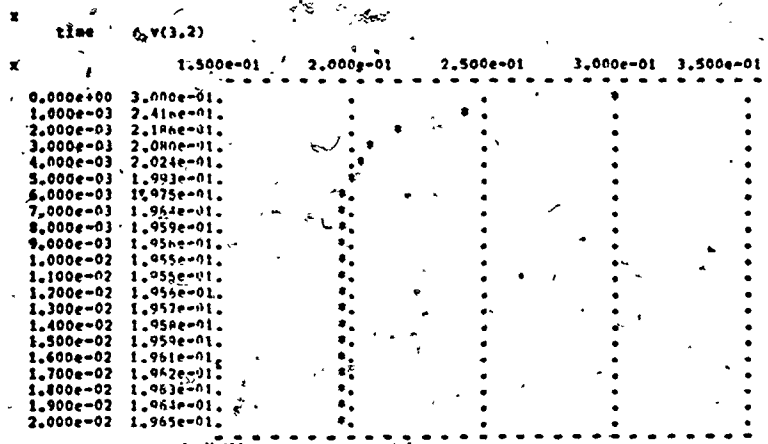
19. Brus 1.4nl Distributed reaction-diffusion circuit (tetrahedron topology schematic Figure 4); same as Brus 1.4n, but sources in volume 4 only, isb pulsed once.

20. Spice program for plot 5, Brus 1.4c (series topology schematic Figure 4).*

*All Spice programs were run on a VAX 11/780 under the UNIX operating system.

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Plot 1



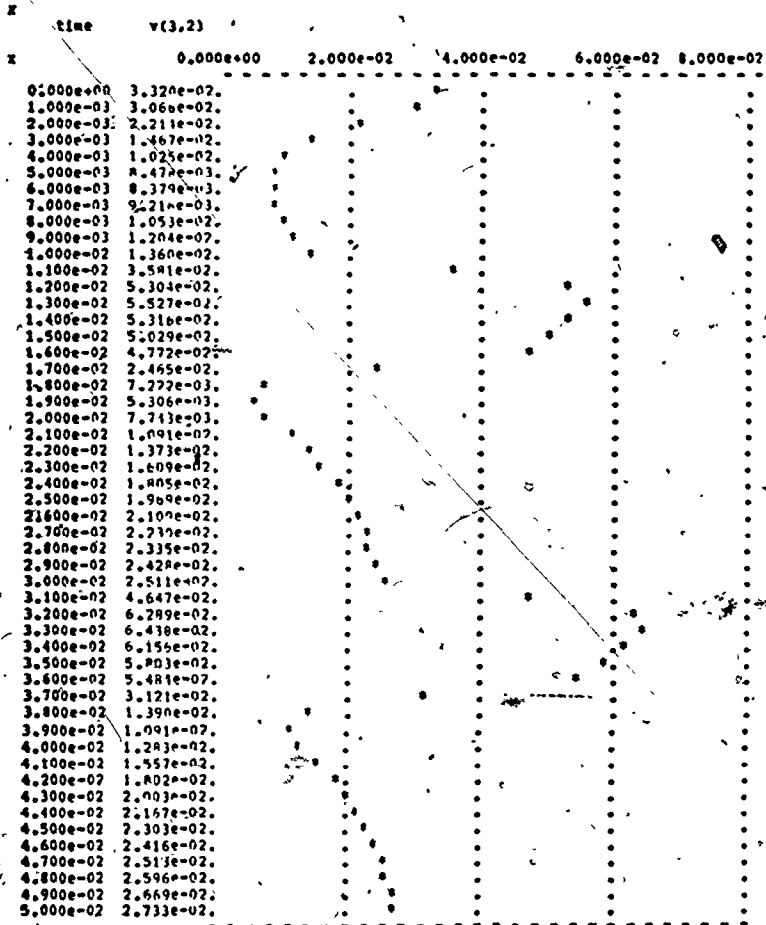
***** S ***** Spice 2.Xz (vax/1/780) *****

Plot 2

0.hrdsl.4a

***** Transient Analysis

temperature = 25.000 deg c



00000 transient analysis temperature = 25.000 deg c

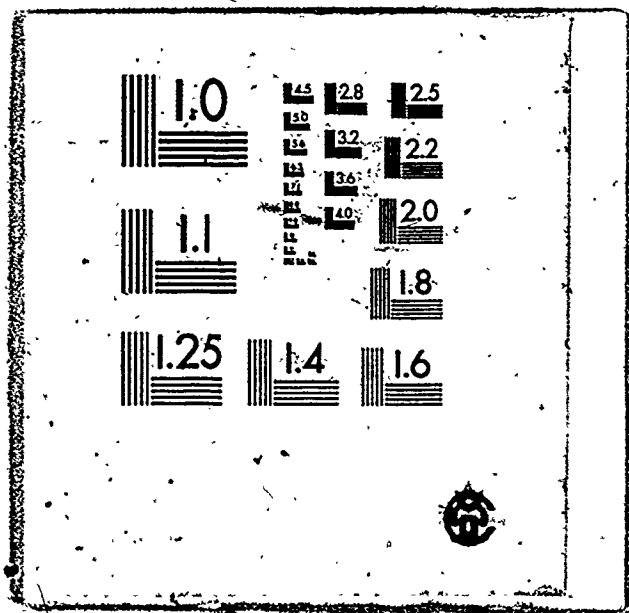
z time v(3,2) Plot 3

z	0.000e+00	2.000e-02	4.000e-02	6.000e-02	8.000e-02
0.000e+00	3.320e-02				
1.000e-03	3.146e-02				
2.000e-03	2.505e-02				
3.000e-03	1.864e-02				
4.000e-03	1.432e-02				
5.000e-03	1.205e-02				
6.000e-03	1.132e-02				
7.000e-03	1.156e-02				
8.000e-03	1.236e-02				
9.000e-03	1.344e-02				
1.000e-02	1.466e-02				
1.100e-02	1.605e-02				
1.200e-02	1.502e-02				
1.300e-02	7.274e-02				
1.400e-02	7.324e-02				
1.500e-02	7.094e-02				
1.600e-02	6.794e-02				
1.700e-02	4.655e-02				
1.800e-02	1.375e-02				
1.900e-02	4.915e-03				
2.000e-02	3.415e-03				
2.100e-02	4.772e-03				
2.200e-02	6.923e-03				
2.300e-02	9.167e-03				
2.400e-02	1.124e-02				
2.500e-02	1.321e-02				
2.600e-02	1.445e-02				
2.700e-02	1.652e-02				
2.800e-02	1.794e-02				
2.900e-02	1.927e-02				
3.000e-02	2.034e-02				
3.100e-02	4.557e-02				
3.200e-02	6.972e-02				
3.300e-02	7.720e-02				
3.400e-02	7.775e-02				
3.500e-02	7.537e-02				
3.600e-02	7.200e-02				
3.700e-02	4.430e-02				
3.800e-02	1.731e-02				
3.900e-02	4.233e-03				
4.000e-02	6.499e-03				
4.100e-02	7.640e-03				
4.200e-02	9.590e-03				
4.300e-02	1.165e-02				
4.400e-02	1.359e-02				
4.500e-02	1.535e-02				
4.600e-02	1.695e-02				
4.700e-02	1.838e-02				
4.800e-02	1.967e-02				
4.900e-02	2.084e-02				
5.000e-02	2.190e-02				

transient analysis temperature = 25,000 deg c
 Plot 4

time	v(3,2)				
		0.000e+00	2.000e-02	4.000e-02	6.000e-02
0.000e+00	1.320e-02				
1.000e-03	1.140e-02				
2.000e-03	2.505e-02				
3.000e-03	1.869e-02				
4.000e-03	1.432e-02				
5.000e-03	1.205e-02				
6.000e-03	1.132e-02				
7.000e-03	1.150e-02				
8.000e-03	1.236e-02				
9.000e-03	1.343e-02				
1.000e-02	1.460e-02				
1.100e-02	4.005e-02				
1.200e-02	6.500e-02				
1.300e-02	7.274e-02				
1.400e-02	7.325e-02				
1.500e-02	7.090e-02				
1.600e-02	6.799e-02				
1.700e-02	4.055e-02				
1.800e-02	1.375e-02				
1.900e-02	4.910e-01				
2.000e-02	3.415e-01				
2.100e-02	4.772e-01				
2.200e-02	6.923e-01				
2.300e-02	9.147e-01				
2.400e-02	1.124e-02				
2.500e-02	1.321e-02				
2.600e-02	1.495e-02				
2.700e-02	1.652e-02				
2.800e-02	1.794e-02				
2.900e-02	1.922e-02				
3.000e-02	2.048e-02				
3.100e-02	2.144e-02				
3.200e-02	2.240e-02				
3.300e-02	2.328e-02				
3.400e-02	2.409e-02				
3.500e-02	2.483e-02				
3.600e-02	2.550e-02				
3.700e-02	2.612e-02				
3.800e-02	2.669e-02				
3.900e-02	2.722e-02				
4.000e-02	2.770e-02				
4.100e-02	2.815e-02				
4.200e-02	2.856e-02				
4.300e-02	2.893e-02				
4.400e-02	2.929e-01				
4.500e-02	2.961e-02				
4.600e-02	2.991e-02				
4.700e-02	3.018e-02				
4.800e-02	3.044e-02				
4.900e-02	3.067e-02				
5.000e-02	3.089e-02				

2 OF / DE 2



< 0,brus1,4r2
***** transient analysis ***** temperature = 25.000 deg.c

Plot-7
Legend:

*1 v(31,21)
*2 v(32,22)
*3 v(33,23)
*4 v(34,24)

time v(31,21)

x(*)----- 0.000e+00 2.000e-02 4.000e-02 6.000e-02 8.000e-02

x(+)----- -5.000e-02 0.000e+00 5.000e-02 1.000e-01 1.500e-01

x(s)----- -1.500e-01 -1.000e-01 -5.000e-02 0.000e+00 5.000e-02

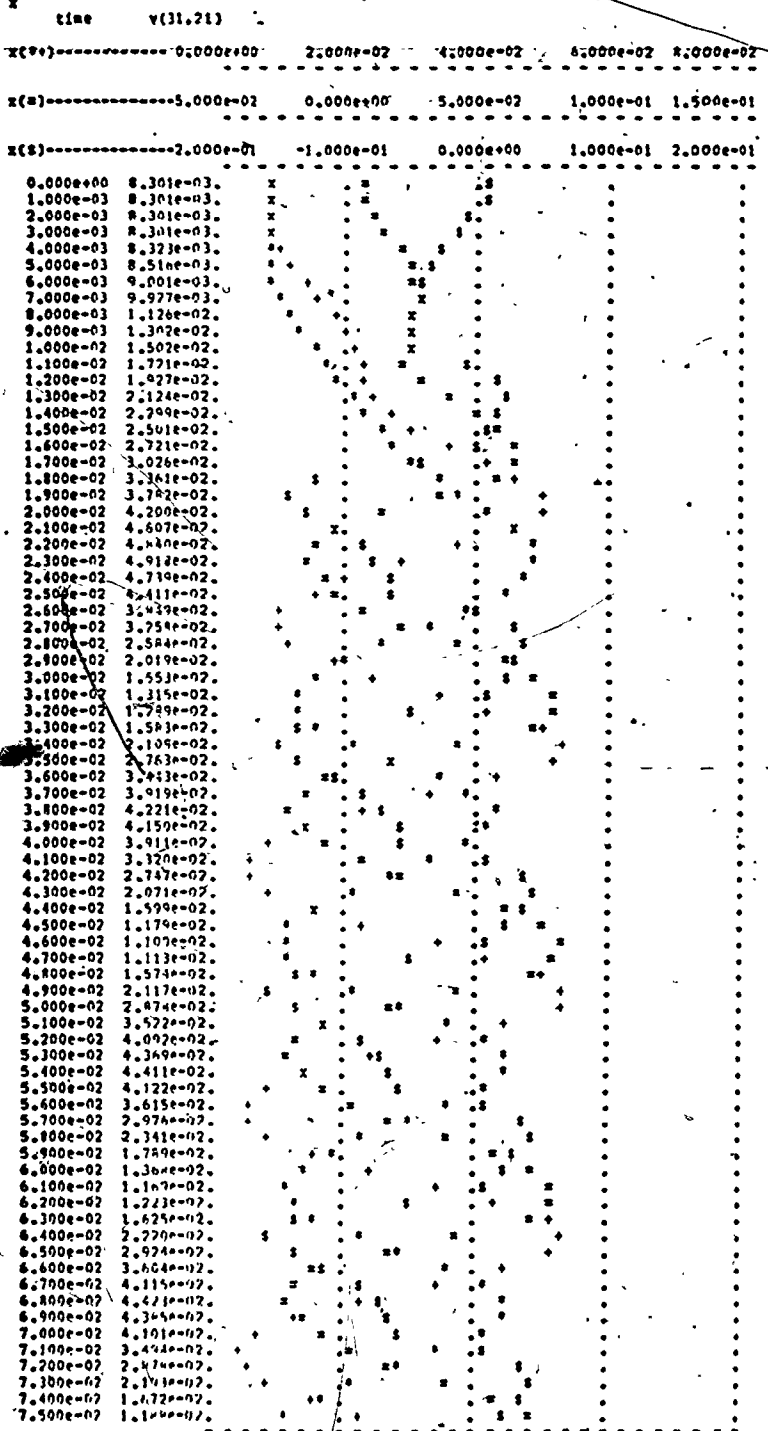
time	v(31,21)	v(32,22)	v(33,23)	v(34,24)
0.000e+00	8.301e-01			
1.000e-03	8.301e-01			
2.000e-03	8.301e-01			
3.000e-03	8.301e-01			
4.000e-03	8.317e-01			
5.000e-03	8.684e-01			
6.000e-03	9.525e-01			
7.000e-03	1.108e-01			
8.000e-03	1.314e-02			
9.000e-03	1.560e-02			
1.000e-02	1.794e-02			
1.100e-02	1.990e-02			
1.200e-02	2.090e-02			
1.300e-02	2.150e-02			
1.400e-02	2.194e-02			
1.500e-02	2.293e-02			
1.600e-02	2.446e-02			
1.700e-02	2.676e-02			
1.800e-02	3.352e-02			
1.900e-02	3.902e-02			
2.000e-02	4.302e-02			
2.100e-02	4.747e-02			
2.200e-02	4.771e-02			
2.300e-02	4.477e-02			
2.400e-02	3.832e-02			
2.500e-02	3.043e-02			
2.600e-02	2.270e-02			
2.700e-02	1.612e-02			
2.800e-02	1.235e-02			
2.900e-02	1.140e-02			
3.000e-02	1.252e-02			
3.100e-02	1.460e-02			
3.200e-02	1.640e-02			
3.300e-02	1.856e-02			
3.400e-02	2.000e-02			
3.500e-02	2.050e-02			
3.600e-02	2.140e-02			
3.700e-02	2.174e-02			
3.800e-02	2.107e-02			
3.900e-02	2.344e-02			
4.000e-02	2.501e-02			
4.100e-02	2.514e-02			
4.200e-02	2.430e-02			
4.300e-02	2.569e-02			
4.400e-02	2.624e-02			
4.500e-02	2.503e-02			
4.600e-02	2.520e-02			
4.700e-02	2.309e-02			
4.800e-02	2.421e-02			
4.900e-02	2.311e-02			
5.000e-02	2.376e-02			
5.100e-02	2.307e-02			
5.200e-02	2.404e-02			
5.300e-02	2.306e-02			
5.400e-02	2.470e-02			
5.500e-02	2.454e-02			
5.600e-02	2.543e-02			
5.700e-02	2.540e-02			
5.800e-02	2.637e-02			
5.900e-02	2.600e-02			
6.000e-02	2.670e-02			
6.100e-02	2.657e-02			
6.200e-02	2.776e-02			
6.300e-02	2.644e-02			
6.400e-02	2.740e-02			
6.500e-02	2.690e-02			
6.600e-02	2.770e-02			
6.700e-02	2.641e-02			
6.800e-02	2.724e-02			
6.900e-02	2.670e-02			
7.000e-02	2.711e-02			
7.100e-02	2.641e-02			
7.200e-02	2.704e-02			
7.300e-02	2.660e-02			
7.400e-02	2.704e-02			
7.500e-02	2.660e-02			

00000 transient analysis temperature = 25.000 deg c

0legend:

Plot 8

- *1 v(31,21)
- *2 v(32,22)
- *3 v(33,23)
- *4 v(34,24)



0**** transient analysis

temperature = 25.000 deg c

0legend:

Plot 0

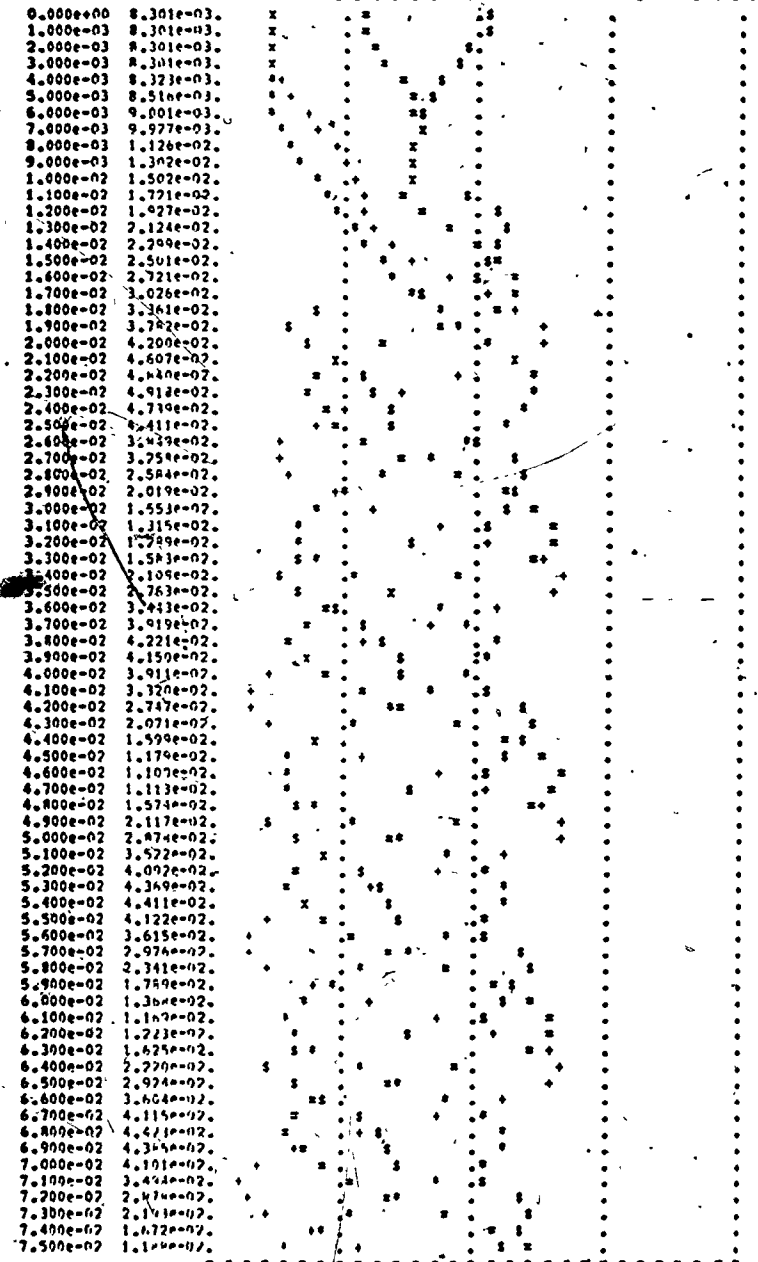
- *1 v(31,21)
- *2 v(32,22)
- *3 v(33,23)
- *4 v(34,24)

x time v(31,21)

x(*)-----0.000e+00 2.000e-02 4.000e-02 6.000e-02 8.000e-02

x(m)-----5.000e-01 0.000e+00 5.000e-02 1.000e-01 1.500e-01

x(s)-----2.000e-01 -1.000e-01 0.000e+00 1.000e-01 2.000e-01



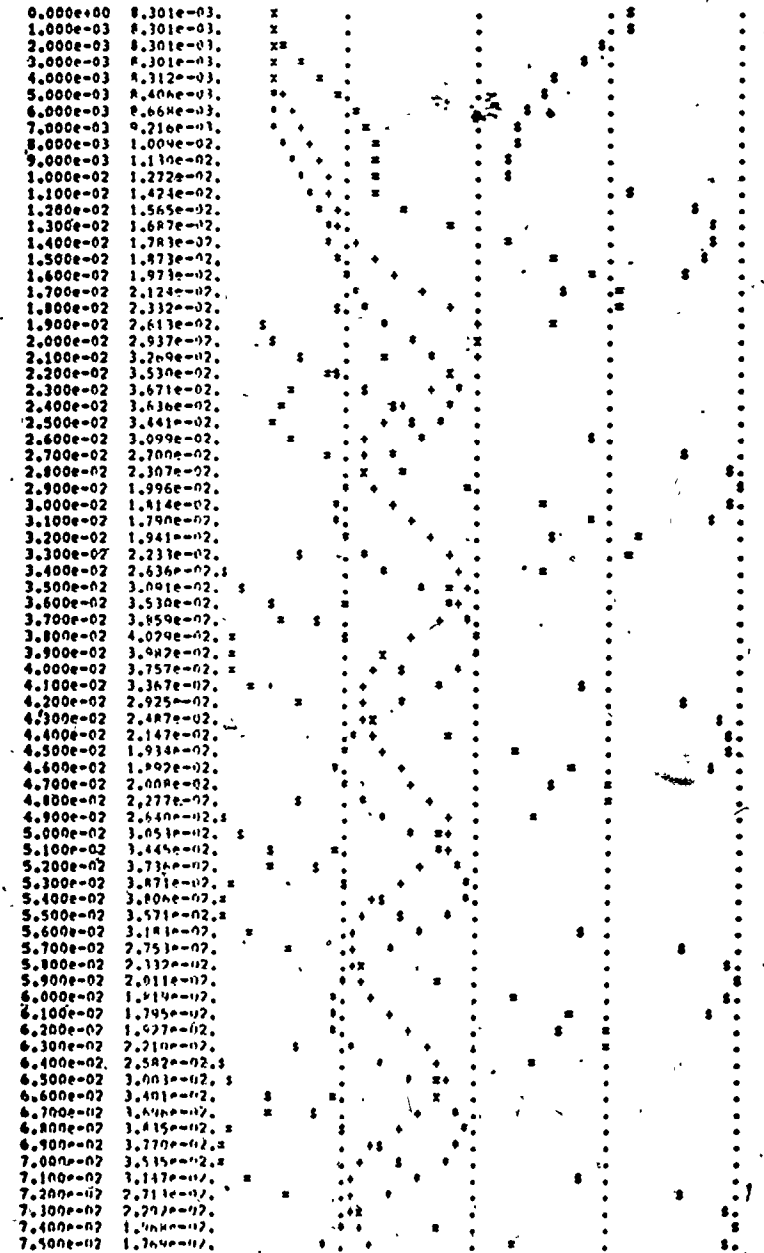
***** transient analysis temperature = 25.000 deg c

01ecndt Plot 10

*1 v(31,21)
*2 v(32,22)
*3 v(33,23)
*4 v(34,24)

x time v(31,21)
x(1+x)----- 0.000e+00 2.000e-02 4.000e-02 6.000e-02 8.000e-02

x(2)----- -1.500e-01 -1.000e-01 -5.000e-02 0.000e+00 5.000e-02



00000 transient analysis

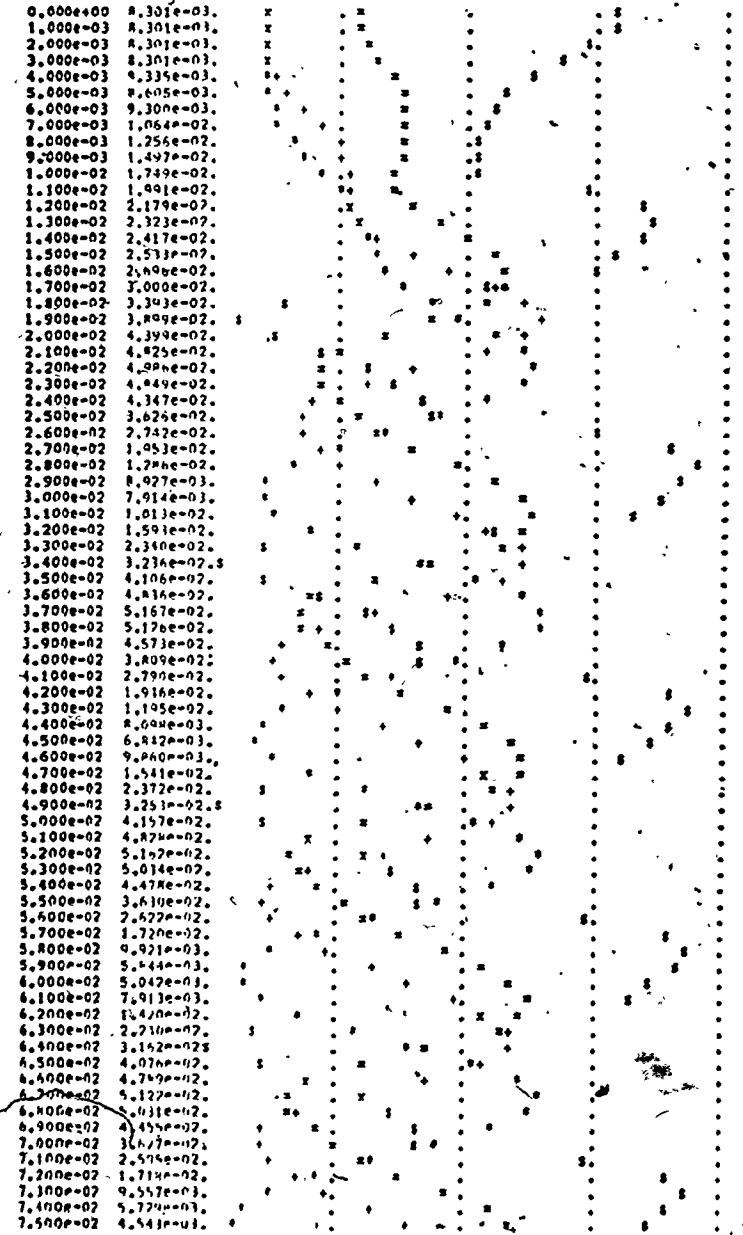
temperature = 75.000 deg c

01e-00001

Plot 11

*1 v(31,21)
*2 v(32,22)
*3 v(33,23)
*4 v(34,24)

time	v(31,21)				
x(*)-----	0.000e+00	2.000e-02	4.000e-02	6.000e-02	8.000e-02
x(m)-----	5.000e-02	0.000e+00	5.000e-02	1.000e-01	1.500e-01
x(S)-----	1.500e-01	-1.000e-01	-5.000e-02	0.000e+00	5.000e-02



**** transient analysis

temperature = 25.000 deg c

Legend:

Plot 12

- o: v(31,21)
- x: v(32,22)
- u: v(33,23)
- s: v(34,24)

time	v(31,21)	v(32,22)	v(33,23)	v(34,24)
0.000e+00	0.000e+00	1.000e-02	2.000e-02	3.000e-02
0.000e+00	0.000e+00	2.000e-02	4.000e-02	6.000e-02
-2.000e-01	-1.000e-01	0.000e+00	1.000e-01	2.000e-01
0.000e+00	8.301e-03	x	x	s
1.000e-03	8.301e-03	x	x	s
2.000e-03	8.301e-03	x	x	s
3.000e-03	8.301e-03	x	x	s
4.000e-03	8.301e-03	x	x	s
5.000e-03	8.301e-03	x	x	s
6.000e-03	8.301e-03	x	x	s
7.000e-03	8.301e-03	x	x	s
8.000e-03	8.301e-03	x	x	s
9.000e-03	8.302e-03	x	x	s
1.000e-02	8.330e-03	x	x	s
1.100e-02	8.443e-03	x	x	s
1.200e-02	8.748e-03	x	x	s
1.300e-02	9.174e-03	x	x	s
1.400e-02	9.737e-03	x	x	s
1.500e-02	1.040e-02	x	x	s
1.600e-02	1.117e-02	x	x	s
1.700e-02	1.201e-02	x	x	s
1.800e-02	1.277e-02	x	x	s
1.900e-02	1.374e-02	x	x	s
2.000e-02	1.472e-02	x	x	s
2.100e-02	1.561e-02	x	x	s
2.200e-02	1.754e-02	x	x	s
2.300e-02	1.952e-02	x	x	s
2.400e-02	2.174e-02	x	x	s
2.500e-02	2.410e-02	x	x	s
2.600e-02	2.663e-02	x	x	s
2.700e-02	2.846e-02	x	x	s
2.800e-02	3.051e-02	x	x	s
2.900e-02	3.147e-02	x	x	s
3.000e-02	3.190e-02	x	x	s
3.100e-02	3.224e-02	x	x	s
3.200e-02	3.270e-02	x	x	s
3.300e-02	3.183e-02	x	x	s
3.400e-02	3.174e-02	x	x	s
3.500e-02	3.076e-02	x	x	s
3.600e-02	3.061e-02	x	x	s
3.700e-02	3.049e-02	x	x	s
3.800e-02	3.016e-02	x	x	s
3.900e-02	3.029e-02	x	x	s
4.000e-02	3.065e-02	x	x	s
4.100e-02	3.145e-02	x	x	s
4.200e-02	3.197e-02	x	x	s
4.300e-02	3.194e-02	x	x	s
4.400e-02	3.139e-02	x	x	s
4.500e-02	3.074e-02	x	x	s
4.600e-02	3.013e-02	x	x	s
4.700e-02	2.905e-02	x	x	s
4.800e-02	2.767e-02	x	x	s
4.900e-02	2.617e-02	x	x	s
5.000e-02	2.533e-02	x	x	s
5.100e-02	2.517e-02	x	x	s
5.200e-02	2.575e-02	x	x	s
5.300e-02	2.475e-02	x	x	s
5.400e-02	2.503e-02	x	x	s
5.500e-02	2.576e-02	x	x	s
5.600e-02	2.694e-02	x	x	s
5.700e-02	2.754e-02	x	x	s
5.800e-02	2.750e-02	x	x	s
5.900e-02	2.699e-02	x	x	s
6.000e-02	2.665e-02	x	x	s
6.100e-02	2.653e-02	x	x	s
6.200e-02	2.572e-02	x	x	s
6.300e-02	2.463e-02	x	x	s
6.400e-02	2.355e-02	x	x	s
6.500e-02	2.327e-02	x	x	s
6.600e-02	2.316e-02	x	x	s
6.700e-02	2.310e-02	x	x	s
6.800e-02	2.379e-02	x	x	s
6.900e-02	2.347e-02	x	x	s
7.000e-02	2.458e-02	x	x	s
7.100e-02	2.617e-02	x	x	s
7.200e-02	2.699e-02	x	x	s
7.300e-02	2.648e-02	x	x	s
7.400e-02	2.673e-02	x	x	s
7.500e-02	2.693e-02	x	x	s

transient analysis temperature = 25,000 deg c

elements

Plot 13

o2 v(31,21)
o1 v(32,22)
o3 v(33,23)
o4 v(34,24)

time	v(31,21)	v(32,22)	v(33,23)	v(34,24)
0.000e+00	3.320e-02			
1.000e-03	3.042e-02			
2.000e-03	2.371e-02			
3.000e-03	1.747e-02			
4.000e-03	1.251e-02			
5.000e-03	1.004e-02			
6.000e-03	8.874e-03			
7.000e-03	9.239e-03			
8.000e-03	9.727e-03			
9.000e-03	1.062e-02			
1.000e-02	1.137e-02			
1.100e-02	1.200e-02			
1.200e-02	1.259e-02			
1.300e-02	1.315e-02			
1.400e-02	1.370e-02			
1.500e-02	1.424e-02			
1.600e-02	1.476e-02			
1.700e-02	1.527e-02			
1.800e-02	1.577e-02			
1.900e-02	1.626e-02			
2.000e-02	1.674e-02			
2.100e-02	1.721e-02			
2.200e-02	1.767e-02			
2.300e-02	1.812e-02			
2.400e-02	1.857e-02			
2.500e-02	1.901e-02			
2.600e-02	1.944e-02			
2.700e-02	1.987e-02			
2.800e-02	2.029e-02			
2.900e-02	2.071e-02			
3.000e-02	2.112e-02			
3.100e-02	2.153e-02			
3.200e-02	2.194e-02			
3.300e-02	2.234e-02			
3.400e-02	2.274e-02			
3.500e-02	2.314e-02			
3.600e-02	2.353e-02			
3.700e-02	2.392e-02			
3.800e-02	2.431e-02			
3.900e-02	2.470e-02			
4.000e-02	2.508e-02			
4.100e-02	2.546e-02			
4.200e-02	2.584e-02			
4.300e-02	2.622e-02			
4.400e-02	2.659e-02			
4.500e-02	2.696e-02			
4.600e-02	2.733e-02			
4.700e-02	2.770e-02			
4.800e-02	2.807e-02			
4.900e-02	2.844e-02			
5.000e-02	2.881e-02			
5.100e-02	2.918e-02			
5.200e-02	2.955e-02			
5.300e-02	2.992e-02			
5.400e-02	3.029e-02			
5.500e-02	3.066e-02			
5.600e-02	3.103e-02			
5.700e-02	3.140e-02			
5.800e-02	3.177e-02			
5.900e-02	3.214e-02			
6.000e-02	3.251e-02			
6.100e-02	3.288e-02			
6.200e-02	3.325e-02			
6.300e-02	3.362e-02			
6.400e-02	3.399e-02			
6.500e-02	3.436e-02			
6.600e-02	3.473e-02			
6.700e-02	3.510e-02			
6.800e-02	3.547e-02			
6.900e-02	3.584e-02			
7.000e-02	3.621e-02			
7.100e-02	3.658e-02			
7.200e-02	3.695e-02			
7.300e-02	3.732e-02			
7.400e-02	3.769e-02			
7.500e-02	3.806e-02			

00000 transient analysis. temperature = 25.000 deg c

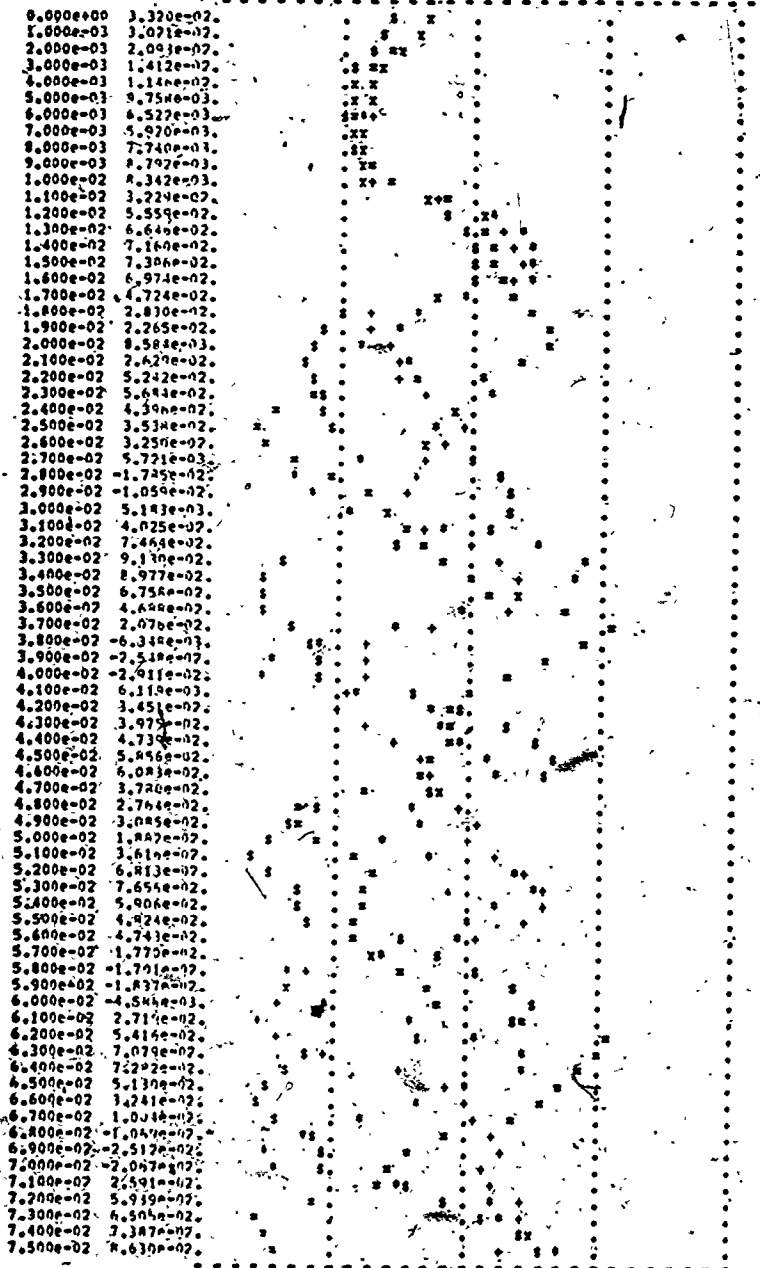
01elements Plot 14

* v(31,21)
* v(32,22)
* v(33,23)
* v(34,24)

X time v(31,21)

x(0+s)-----5.000e-02 0.000e+00 5.000e-02 1.000e-01 1.500e-01

x(s)-----1.000e-01 0.000e+00 1.000e-01 2.000e-01 3.000e-01

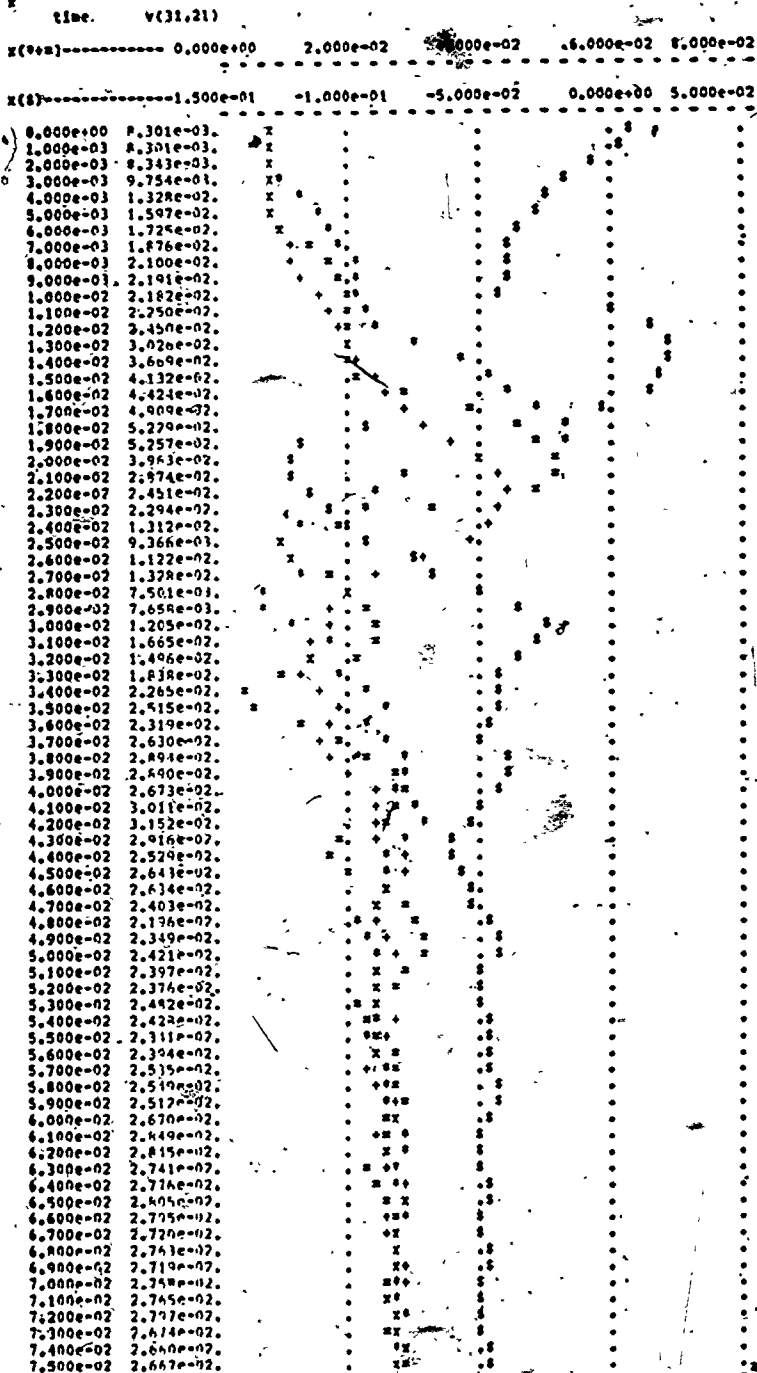


00000 transient analysis temperature = 25.000 deg c

Legend:

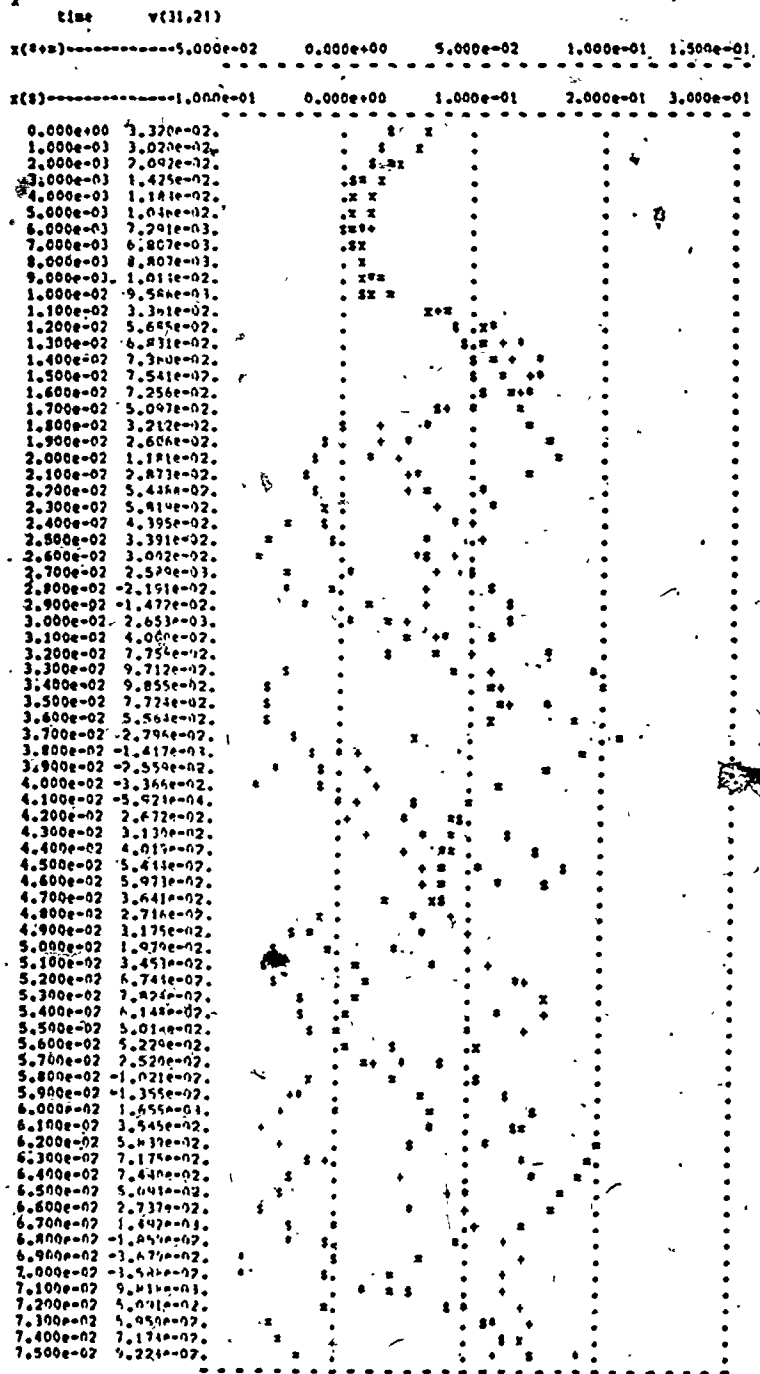
Plot 15

v(31,21)
v(32,27)
v(33,23)
st.v(34,24)



***** transient Analysis temperature = 25.000 deg c
Plot 18

Legend:
S1 v(31,21)
S2 v(32,22)
S3 v(33,23)
S4 v(34,24)
X



00000 transient analysis temperature = 25.000 deg c

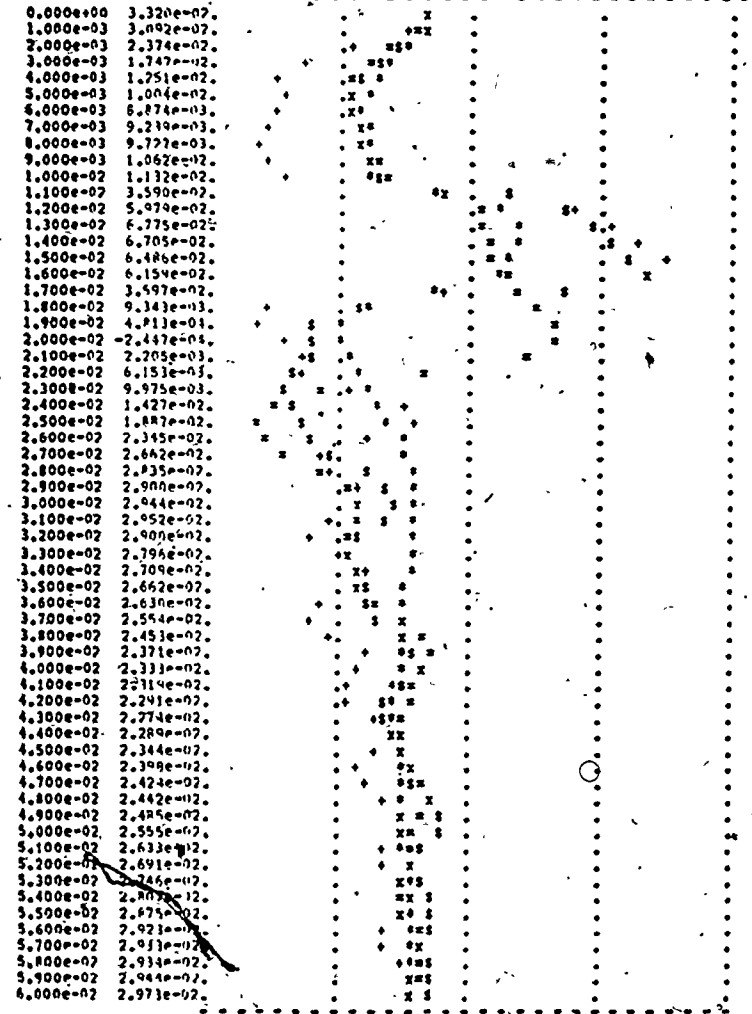
0legends

Plot 17

- *1 v(31,21)
- *2 v(32,72)
- *3 v(33,73)
- *4 v(34,24)

X
time v(31,21)
x(us)-----5.000e-02 0.000e+00 5.000e-02 1.000e-01 1.500e-01

x(+)------0.000e+00 2.000e-02 4.000e-02 6.000e-02 8.000e-02



00000 transient analysis

temperature = 25.000 deg c

0 legends:

Plot 18

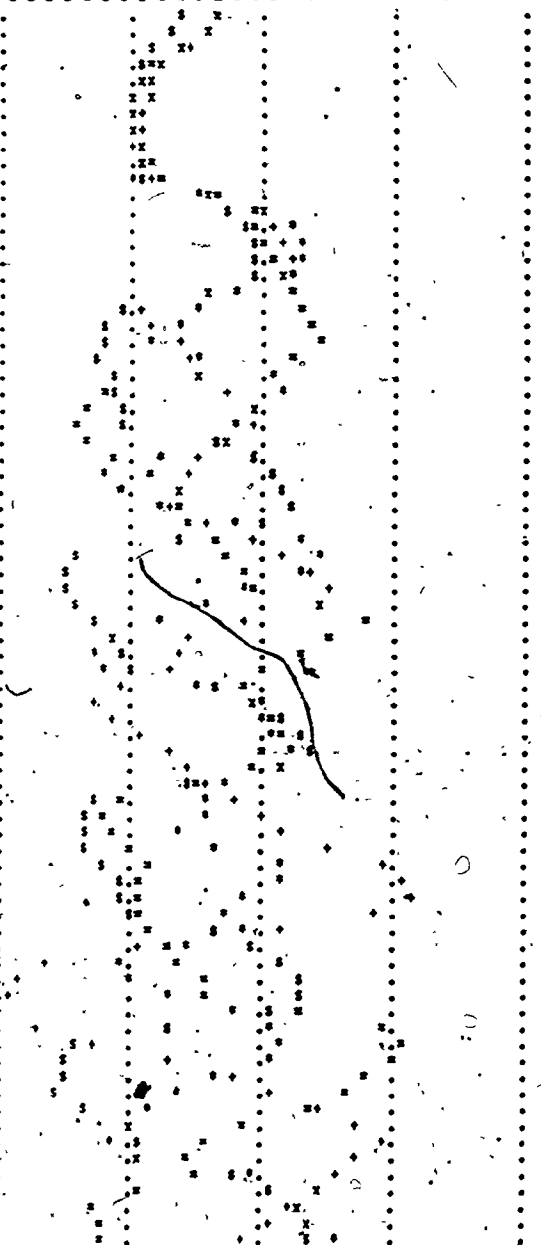
- *1 v(31,21)
- *2 v(32,22)
- *3 v(33,23)
- *4 v(34,24)

x time v(31,21)

x(100)-----5.000e-02 0.000e+00 5.000e-02 1.000e-01 1.500e-01

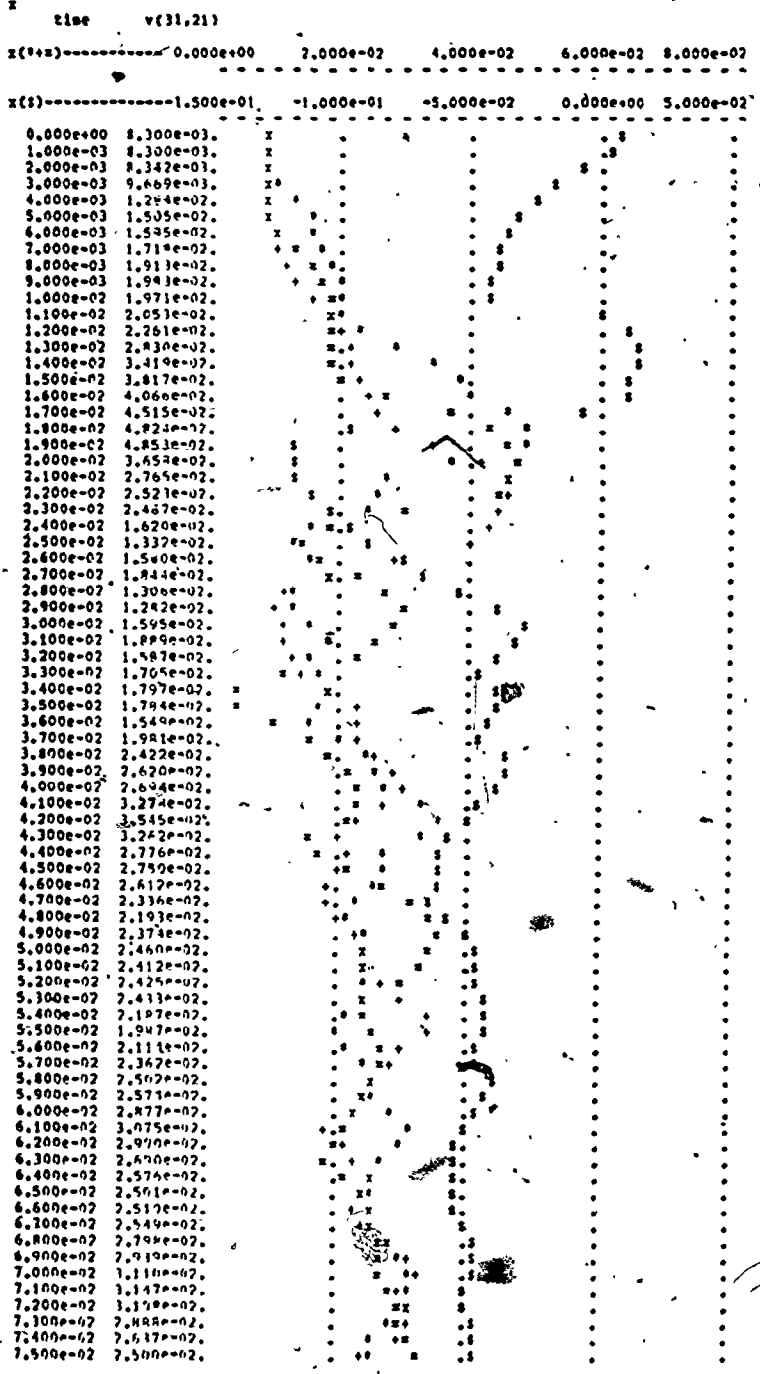
x(1)-----1.000e-01 0.000e+00 1.000e-01 2.000e-01 3.000e-01

0.000e+00 1.320e-02
 1.000e-03 2.944e-07
 2.000e-03 1.451e-02
 3.000e-03 1.106e-02
 4.000e-03 8.019e-03
 5.000e-03 5.420e-03
 6.000e-03 1.678e-03
 7.000e-03 7.052e-04
 8.000e-03 2.020e-03
 9.000e-03 7.517e-03
 1.000e-02 1.643e-03
 1.100e-02 2.552e-02
 1.200e-02 4.416e-02
 1.300e-02 5.906e-02
 1.400e-02 6.464e-02
 1.500e-02 6.570e-02
 1.600e-02 6.241e-02
 1.700e-02 4.073e-02
 1.800e-02 2.354e-07
 1.900e-02 1.807e-02
 2.000e-02 6.354e-03
 2.100e-02 2.637e-12
 2.200e-02 5.341e-02
 2.300e-02 5.714e-07
 2.400e-02 4.490e-02
 2.500e-02 3.901e-02
 2.600e-02 3.640e-02
 2.700e-02 1.077e-12
 2.800e-02 -1.118e-07
 2.900e-02 -4.487e-03
 3.000e-02 8.939e-03
 3.100e-02 3.922e-02
 3.200e-02 6.525e-02
 3.300e-02 7.220e-02
 3.400e-02 6.478e-07
 3.500e-02 4.256e-07
 3.600e-02 2.750e-02
 3.700e-02 9.746e-03
 3.800e-02 -4.403e-03
 3.900e-02 -1.582e-02
 4.000e-02 -1.102e-02
 4.100e-02 2.584e-02
 4.200e-02 4.631e-02
 4.300e-02 4.448e-02
 4.400e-02 5.243e-02
 4.500e-02 5.317e-02
 4.600e-02 5.604e-02
 4.700e-02 3.624e-07
 4.800e-02 2.804e-02
 4.900e-02 2.975e-02
 5.000e-02 1.650e-02
 5.100e-02 3.180e-07
 5.200e-02 5.596e-02
 5.300e-02 5.272e-02
 5.400e-02 4.161e-02
 5.500e-02 1.742e-02
 5.600e-02 4.197e-02
 5.700e-02 2.193e-07
 5.800e-02 -3.694e-03
 5.900e-02 3.413e-04
 6.000e-02 1.249e-02
 6.100e-02 3.780e-07
 6.200e-02 5.216e-02
 6.300e-02 5.203e-02
 6.400e-02 5.347e-02
 6.500e-02 3.074e-02
 6.600e-02 1.429e-02
 6.700e-02 7.531e-03
 6.800e-02 2.151e-04
 6.900e-02 -4.457e-03
 7.000e-02 3.800e-03
 7.100e-02 4.681e-02
 7.200e-02 7.057e-07
 7.300e-02 4.417e-02
 7.400e-02 4.790e-02
 7.500e-02 7.757e-02



00000 transient Analysis - Temperature = 25.000 deg C
Plot 10

01e2nd: 2
* v(31,21)
* v(32,22)
* v(33,23)
* v(34,24)



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.brus1.4c

Plot 20

*Distributed reaction-diffusion circuit:
 *series connection of volume subcircuits, vol4 sources, equal impedances
 *and time delays, plot cx's, non-linear

tx1 0 31 0 32 z0=1 td=.001s
 tx2 0 32 0 33 z0=1 td=.001s
 tx3 0 33 0 34 z0=1 td=.001s
 ty1 0 71 0 72 z0=1 td=.001s
 ty2 0 72 0 73 z0=1 td=.001s
 ty3 0 73 0 74 z0=1 td=.001s
 x1 21 31 71 vol1
 x2 22 32 72 vol2
 x3 23 33 73 vol3
 x4 24 34 74 vol4

.subckt vol1 21 31 71
 *isa 0 1 pulse (.1 1 0 0 200s 200s)
 *isb 0 12 pulse (0 1 .01s .001s .001s .005s .010s)
 vse 4 0 0
 vsd 9 0 0
 ca 1 21 .0048 ic=.1
 cb 12 5 .0048 ic=.1
 ce 4 21 .0048 ic=.1
 cd 9 8 .0048 ic=.1
 cx 31 21 .014 ic=.3
 cy 71 21 .0048 ic=.1
 d1 31 5 dmod1
 d2 31 6 dmod2
 d3 12 11 dmod3
 d4 9 10 dmod3a
 d5 71 6 dmod4
 d6 71 8 dmod5
 d7 13 31 dmod6
 r1 31 1 1
 r2 31 4 1
 *r3 11 10 1
 qlvccs 11 10 11 10 1m 1m
 *r4 6 13 1
 qvccs 6 13 6 13 1m 1m 1m 1m
 rg1 1 0 1
 rg2 21 0 1000
 rg3 31 0 1000
 rg4 4 0 1
 rg5 5 0 1000
 rg6 6 0 1000
 rg7 71 0 1000
 rg8 8 0 1000
 rg9 9 0 1
 rg10 10 0 1000
 rg11 11 0 1000
 rg12 12 0 1
 rg13 13 0 1000
 .model dmod1 d(is=1 n=1.1 rs=.025)
 .model dmod2 d(is=2 n=2 rs=.25)

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```
.model dmod3 d(is=1 n=1 rs=.048)
.model dmod3a d(is=1 n=1 rs=.07)
.model dmod4 d(is=1 n=1 rs=.08)
.model dmod5 d(is=1 n=1.2 rs=.03)
.model dmod6 d(is=3 n=3 rs=.15)
.ends vol1
```

```
.subckt vol2 22 32 72
*isa 0 1 pulse (.1 1 0 0 200s 200s)
*isb 0 12 pulse (0 1 .01s .001s .001s .005s .020s)
vse 4 0 0
vsd 9 0 0
ca 1 22 .0048 ic=.1
cb 12 5 .0048 ic=.1
ce 4 22 .0048 ic=.1
cd 9 8 .0048 ic=.1
cx 32 22 .014 ic=.3
cy 72 22 .0048 ic=.1
d1 32 5 dmod1
d2 32 6 dmod2
d3 12 11 dmod3
d4 9 10 dmod3a
d5 72 6 dmod4
d6 72 8 dmod5
d7 13 32 dmod6
r1 32 1 1
r2 32 4 1
*r3 11 10 1
qivccs 11 10 11 10 1m 1m
*r4 6 13 1
gvccs 6 13 6 13 1m 1m 1m 1m
rq1 1 0 1
rq2 22 0 1000
rq3 32 0 1000
rq4 4 0 1
rq5 5 0 1000
rq6 6 0 1000
rq7 72 0 1000
rq8 8 0 1000
rq9 9 0 1
rq10 10 0 1000
rq11 11 0 1000
rq12 12 0 1
rq13 13 0 1000
.model dmod1 d(is=1 n=1.1 rs=.025)
.model dmod2 d(is=2 n=2 rs=.25)
.model dmod3 d(is=1 n=1 rs=.048)
.model dmod3a d(is=1 n=1 rs=.07)
.model dmod4 d(is=1 n=1 rs=.08)
.model dmod5 d(is=1 n=1.2 rs=.03)
.model dmod6 d(is=3 n=3 rs=.15)
.ends vol2
```

```
.subckt vol3 23 33 73
*isa 0 1 pulse (.1 1 0 0 200s 200s)
*isb 0 12 pulse (0 1 .01s .001s .001s .01s .015s)
```


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```

vse 4 0 0
vsd 9 0 0
ca 1 23 .0048 ic=.1
cb 12 5 .0048 ic=.1
ce 4 23 .0048 ic=.1
cd 9 8 .0048 ic=.1
cx 33 23 .014 ic=.3
cy 73 23 .0048 ic=.1
d1 33 5 dmod1
d2 33 6 dmod2
d3 12 11 dmod3
d4 9 10 dmod3a
d5 73 6 dmod4
d6 73 8 dmod5
d7 13 33 dmod6
r1 33 1 1
r2 33 4 1
*r3 11 10 1
qlvccs 11 10 11 10 1m 1m
*r4 6 13 1
qvccs 6 13 6 13 1m 1m 1m 1m
rq1 1 0 1
rq2 23 0 1000
rq3 33 0 1000
rq4 4 0 1
rq5 5 0 1000
rq6 6 0 1000
rq7 73 0 1000
rq8 8 0 1000
rq9 9 0 1
rq10 10 0 1000
rq11 11 0 1000
rq12 12 0 1
rq13 13 0 1000
.model dmod1 d(is=1 n=1.1 rs=.025)
.model dmod2 d(is=2 n=2 rs=.75)
.model dmod3 d(is=1 n=1 rs=.048)
.model dmod3a d(is=1 n=1 rs=.07)
.model dmod4 d(is=1 n=1 rs=.08)
.model dmod5 d(is=1 n=1.2 rs=.03)
.model dmod6 d(is=3 n=3 rs=.15)
.ends vol3

.subckt vol4 24 34 74
isa 0 1 pulse (.1 1 0 0 0 200s 200s)
isb 0 12 pulse (0 5 .01s .001s .001s .005s .015s)
vse 4 0 0
vsd 9 0 0
ca 1 24 .0048 ic=.1
cb 12 5 .0048 ic=.1
ce 4 24 .0048 ic=.1
cd 9 8 .0048 ic=.1
cx 34 24 .014 ic=.3
cy 74 24 .0048 ic=.1
d1 34 5 dmod1
d2 34 6 dmod2

```

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```
d3 12 11 dmod3
d4 9 10 dmod3a
d5 74 6 dmod4
d6 74 8 dmod5
d7 13 34 dmod6
rd 34 1 1
r2 34 4 1
*r3 11 10 1
glvccs 11 10 11 10 1m 1m
*r4 6 13 1
gvccs 6 13 6 13 1m 1m 1m 1m
rg1 1 0 1
rg2 24 0 1000
rg3 34 0 1000
rg4 4 0 1
rg5 5 0 1000
rg6 6 0 1000
rg7 74 0 1000
rg8 8 0 1000
rg9 9 0 1
rg10 10 0 1000
rg11 11 0 1000
rg12 12 0 1
rg13 13 0 1000
.model dmod1 d(is=1 n=1.1 rs=.025)
.model dmod2 d(is=2 n=2 rs=.25)
.model dmod3 d(is=1 n=1 rs=.048)
.model dmod3a d(is=1 n=1 rs=.07)
.model dmod4 d(is=1 n=1 rs=.08)
.model dmod5 d(is=1 n=1.2 rs=.03)
.model dmod6 d(is=3 is=3 rs=.15)
.ends vol4

.width 80=in 80=out
.options reltol=.01 abstol=1.0e-6amp vntol=1.0e-3volt
+ chatol=1.0e-10 limpts=2000 limtim=10.1vlim=2
* noacct nopage nomod nonode
.tran .001s .075s
.plot tran v(31,21) v(32,22) v(33,23) v(34,24)
.end
```

5. Note on Network Modelling of Morphogenesis

Morphogenesis is the differentiation of an organism into characteristic form during the course of its development. The heterogeneity of morphogenetic events and the associated interactions between structure and physiology present difficulties for model building and analysis. Models based on network thermodynamics can include both structural and physiological aspects reduced to the common form of the equivalent circuit. Modelling the morphogenesis of organisms using networks then becomes abstracted to the analogous problem of directed change over time in the topology and parameters of the thermodynamic network model.*

Changes in the morphogenetic system can be classified as either structural or functional in keeping with the customary distinctions used in biology. At the molecular level these distinctions blur.

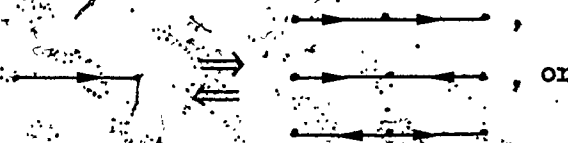
Structural changes can be divided into: (1) change in shape or volume without change in discernible partitions; (2) change in the number of discernible partitions; (3) changes in connections between discernible partitions with or without change in numbers of partitions.

*The use of topological graph models to describe the abstract development of organisms was first suggested by Rashevsky (1954) and extended by him subsequently in a series of papers in the Bulletin of Mathematical Biophysics on "organismic sets". A range of examples of more recent approaches including graph and automata based models can be found in IEEE Conference on Biologically Motivated Automata Theory.

Types of functional changes are: (1) change in values of existing parameters; (2) change in boundary conditions (sources); (3) change in the number of discernible functional components (in analogy with compartments in biological systems); (4) change in the number of types of discernible functional components.

To construct network models of morphogenesis requires that these changes be translated into network representations. Consider an arbitrary initial network with state and boundary values specified at $t = 0$. Production rules guiding change in network structure without consideration of branch parameters (after use in graph grammars which might be useful for this phase of model construction--Petrov, 1978; Ehrig and Tischer, 1974; Ehrig, 1979) for one port, two terminal branches are of three types: insertion (including substitution), deletion and connection.

Bifurcation of a branch: insertion \Rightarrow ; deletion \Leftarrow



Bifurcation of a node:



Changes in the number of loops in a network (feedback):

connection \Rightarrow ; disconnection \Leftarrow



The same production rules apply to all subgraphs with two terminals no matter how large the internal black box graph might be. Production rules for three or more terminal subgraphs are specified using the set-theoretic operations union, intersection, difference or ring sum with the specification of externally recognized nodes and branches of the subgraphs for each operation.

Changes in function, that is the output values of specified terminals, of a network are accomplished by changing source values (boundary conditions), changing branch parameters--both type and value, and/or changing the number and types of subgraph functions. Functional change therefore may or may not involve structural change.

Specification of a timed sequence of structural and functional production rules are considered to define a morphogenetic automaton. An automaton is represented generally by the quintuple $\langle \mathcal{I}, \mathcal{O}, \mathcal{Q}, \mathcal{F}, \mathcal{R} \rangle$ respectively the input, output, internal state vectors, the transition matrix \mathcal{F} and the relational matrix \mathcal{R} (Kobriniskii and Trakhtenbrot, 1965). For a network automaton described by the state equations (sect. 2.7) $\dot{x} = -A x_1 + B u_1$; $y = C x_e + D u_a$, the quintuple can be given the following interpretation: (\odot indicates matrix product)

$$\begin{array}{ccccccc} \mathcal{Q} & \mathcal{R} & \mathcal{I} \times \mathcal{Q} & \mathcal{O} & \mathcal{F} & \mathcal{I} \times \mathcal{Q} \\ x = [A, B] \odot \begin{bmatrix} x_1 \\ u_1 \end{bmatrix} & ; & y = [C, D] \odot \begin{bmatrix} x_e \\ u_a \end{bmatrix} \end{array}$$

Note that $\mathcal{R} : \mathcal{I} \times \mathcal{Q} \xrightarrow{\odot} \mathcal{Q}$ and $\mathcal{F} : \mathcal{I} \times \mathcal{Q} \xrightarrow{\odot} \mathcal{O}$, so $\langle \mathcal{I}, \mathcal{O}, \mathcal{Q}, \mathcal{R}, \mathcal{F} \rangle = \langle x, y, u, [A, B], [C, D] \rangle$.

The construction of a morphogenetic network automaton may be approached in two ways:

1) evolution of a pattern of structure and parameter settings from sequential application of specified rules without regard for the behavior of the automaton during the prior time steps or its state at an arbitrary initial time t .

2) given initial conditions, evolution of the pattern of structure and parameter settings on the basis of the behavior of the network at each time step over a given time interval by application of specified rules only when appropriate circuit responses occur (sensitivity models). Both approaches require a two-step sequence for each structural and/or functional change(s) in the network--an analysis step and a step involving the application of production rules.

Increase in size of finite systems must eventually approach some limit. In network automata this limit means cessation of change in structure and/or function or the establishment of some stable, limited oscillatory pattern (e.g., the limit cycle). Limits, in keeping with distinctions made in the last paragraph, may be 1) pre-set cessation of application of production rules. For example, an automaton with a closed set of elements may grow only to the point where all elements of the set are incorporated into the structure of the automaton. 2) behavior growth limit. Additional applications of production rules make no difference in the outputs of the automaton below some specified threshold value. This type of constraint may also arise from limiting boundary conditions (environmental constraints) imposed upon the network by its surroundings.

6. Conclusion

The domain analysis of networks using the state variable approach (Section 2) has been discussed as a method for studying thermodynamic systems represented as equivalent circuits. Synthesis of the equivalent circuits is based on four types of similitude: dynamical, dimensional, topological, and mathematical which were considered in Section 3. To demonstrate the use of these notions, the method for constructing an equivalent circuit for a simple chemical reaction-diffusion system was explained in detail in Section 4. The resultant circuit was then analyzed using an electronic circuit simulator, Spice on a VAX 11/780.

This circuit also represents a prototype of a method intended ultimately for the analysis of biological systems, particularly compartmental analysis of intra- and inter-cellular transport systems. The construction of morphogenetic automata outlined in Section 5 provides a means to compare the generation of functional forms by explicitly stated rules with the morphogenesis of form in organisms whose design principles can only be conjectured. If sufficiently developed, thermodynamic network based automata could serve as an adjunct to laboratory methods in the design of plants using cell culture methods, by providing a method for simulation of the interaction between physical fields, cellular morphology and novel genetic components.

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Appendix 1

Sample Spice Printout

This Appendix includes the Spice program and analysis of the circuit diagrammed in Figure 8. The following program description is based upon Dowell et al. (1976).

The input listing gives the types of circuit elements (first argument), circuit topology (second and third arguments), parameter values for circuit branches (fourth argument), values for sources, diode models and instructions for the transient analysis interval and integration time step. The meanings of the entries are as follows. isa and isb are current sources representing inputs of substances A and B respectively. isa supplies a constant bias to the circuit of 1 amp. Source isb supplies a rectified square wave pulse of 1 amp at intervals of 20 seconds. vse and vsd are ammeters which short circuit the system to ground (zero voltage, unimpeded current flow) representing the passive removal of substances D and E from the circuit.

The capacitors representing the reactants and products are prefaced by a "c". The capacitance setting (fourth argument) follows the listing of the positive and negative branch nodes (second and third arguments respectively in the line); "ic" indicates initial conditions for capacitors which Spice reads when given instructions on the transient analysis control card, i.e., an initial state other than the zero state is computed. This particular program is for zero-state and initial condition instructions are ignored. As an example, take the line ca 1 2 .0048 ic = 1. This indicates a capacitor branch representing

substance A has positive node 1, negative node 2, has a capacitance value of .0048 farads and an initial charge of 0.1 amperes.

Diode branches are prefaced by a "d". The values for diode settings are indicated on the model control card; "is" is saturation current; "n" is the emission coefficient; "rs" is the ohmic resistance.

Linear resistors are indicated by an initial "r". gvccs and gvccs are voltage controlled current sources with polynomial expansions of two and four terms respectively. (An * at the beginning of a line instructs Spice to ignore the line, and is a useful device for a complex program where several different constitutive relations are substituted at the same location in the circuit topology for different analyses of the circuit.) "rg's" are the node-to-ground resistances.

The .options card allows one to set various tolerances and house-keeping details of the program when other-than-default settings are desired without having to open and modify the source program.

.print and .plot cards allow one to specify which branch voltages are displayed by Spice and in which format they are displayed.

In the course of performing the transient analysis Spice prints the adjacency (node by branch) matrix and a tabulation of the values specified by the input table for all branch elements. The initial transient solution determines the DC operating point of the circuit with inductors shorted and capacitors opened. The DC analysis determines transient initial conditions. The remainder of the program print out gives the results of the transient analysis for the specified branch voltages for each time step where the branches are indicated by their positive and negative bounding nodes respectively.

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1***** e ***** spice 2.Xx (vax11/780) *****

0.brus1.4b

0**** input listing temperature = 25.000 deg c

0*****

*reaction subcircuit: nonlinear resistors, zero state, print branch voltages
*plot cx

```
isa 0 1 pulse (.1 1 0 0 200s 200s)
isb 0 12 pulse (0 1 .01s .001s .001s .005s .020s)
vse 4 0 0
vsd 9 0 0
ca 1 2 .0048 ic=.1
cb 12 5 .0048 ic=.1
ce 4 2 .0048 ic=.1
cd 9 8 .0048 ic=.1
cx 3 2 .014 ic=.3
cy 7 2 .0048 ic=.1
d1 3 5 dmod1
d2 3 6 dmod2
d3 12 11 dmod3
d4 9 10 dmod3a
d5 7 6 dmod4
d6 7 8 dmod5
d7 13 3 dmod6
r1 3 1 1
r2 3 4 1
*r3 11 10 1
glvccs 11 10 11 10 1m 1m
*r4 6 13 1
gvccs 6 13 6 13 1m 1m 1m 1m
rg1 1 0 1
rg2 2 0 1000
rg3 3 0 1000
rg4 4 0 1
rg5 5 0 1000
rg6 6 0 1000
rg7 7 0 1000
rg8 8 0 1000
rg9 9 0 1
rg10 10 0 1000
rg11 11 0 1000
rg12 12 0 1
rg13 13 0 1000

.width 80=in 80=out
.options reit01=.01 abstol=1.0e-6amp vntol=1.0e-3volt
+ chgtol=1.0e-10 limpts=2000 limtim=10 lvltim=2
+ noacct nopage nomod nonode
.model dmod1 d(is=1 n=1.1 rs=.025)
.model dmod2 d(is=2 n=2 rs=.25)
```

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```

.model dmod3 d(is=1 n=1 rs=.048)
.model dmod3a d(is=1 n=1 rs=.07)
.model dmod4 d(is=1 n=1 rs=.08)
.model dmod5 d(is=1 n=1.2 rs=.03)
.model dmod6 d(is=3 n=3 rs=.15)
.tran .001s .05s
.print tran v(0,1) v(0,12)
.print tran v(1,2) v(12,5) v(4,2) v(9,8)
.print tran v(3,2) v(7,2)
.print tran v(3,5) v(12,11) v(9,10) v(7,8)
.print tran v(13,3) v(3,6) v(7,6)
.print tran v(3,1) v(3,4) v(1,10) v(6,13)
.print tran v(1) v(2) v(3) v(4)
.print tran v(5) v(6) v(7) v(8)
.print tran v(9) v(10) v(11) v(12) v(13)
.plot tran v(3,2)
.end

```

0**** circuit element summary temperature = 25.000 deg c

0**** resistors

0	name	nodes	value	tc1	tc2
	r1	3 1	1.00e+00	0.00e+00	0.00e+00
	r2	3 4	1.00e+00	0.00e+00	0.00e+00
	rg1	1 0	1.00e+00	0.00e+00	0.00e+00
	rg2	2 0	1.00e+03	0.00e+00	0.00e+00
	rg3	3 0	1.00e+03	0.00e+00	0.00e+00
	rg4	4 0	1.00e+00	0.00e+00	0.00e+00
	rg5	5 0	1.00e+03	0.00e+00	0.00e+00
	rg6	6 0	1.00e+03	0.00e+00	0.00e+00
	rg7	7 0	1.00e+03	0.00e+00	0.00e+00
	rg8	8 0	1.00e+03	0.00e+00	0.00e+00
	rg9	9 0	1.00e+00	0.00e+00	0.00e+00
	rg10	10 0	1.00e+03	0.00e+00	0.00e+00
	rg11	11 0	1.00e+03	0.00e+00	0.00e+00
	rg12	12 0	1.00e+00	0.00e+00	0.00e+00
	rg13	13 0	1.00e+03	0.00e+00	0.00e+00

0**** capacitors and inductors

0	name	nodes	in cond	value
	ca	1 2	1.00e-01	4.80e-03
	cb	12 5	1.00e-01	4.80e-03
	ce	4 2	1.00e-01	4.80e-03
	cd	9 8	1.00e-01	4.80e-03
	cx	3 2	3.00e-01	1.40e-02
	cy	7 2	1.00e-01	4.80e-03

0**** voltage-controlled current sources

0	name	+	-	dimension	function
---	------	---	---	-----------	----------

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```

glvccs 11 10 1 poly
gvccs 6 13 1 poly
    
```

0**** independent sources

0	name	nodes	dc value	ac value	ac phase	transient
---	------	-------	----------	----------	----------	-----------

vse	4	0	0.00e+00	0.00e+00	0.00e+00	
vsd	9	0	0.00e+00	0.00e+00	0.00e+00	
isa	0	1	1.00e-01	0.00e+00	0.00e+00	pulse
						initial value 1.00e-01
						pulsed value 1.00e+00
						delay time... 0.00e+00
						risetime..... 1.00e-03
						falltime..... 2.00e+02
						width..... 2.00e+02
						period..... 4.00e+02

isb	0	12	0.00e+00	0.00e+00	0.00e+00	pulse
						initial value 0.00e+00
						pulsed value 1.00e+00
						delay time... 1.00e-02
						risetime..... 1.00e-03
						falltime..... 1.00e-03
						width..... 5.00e-03
						period..... 2.00e-02

0**** diodes

0	name	+	-	model	area
	d1	3	5	dmod1	1.000
	d2	3	6	dmod2	1.000
	d3	12	11	dmod3	1.000
	d4	9	10	dmod3a	1.000
	d5	7	6	dmod4	1.000
	d6	7	8	dmod5	1.000
	d7	13	3	dmod6	1.000

0**** initial transient solution temperature = 25.000 deg c

node	voltage	node	voltage	node	voltage	node	voltage
(1)	.0666	(2)	.0000	(3)	.0332	(4)	.0000
(5)	.0332	(6)	.0329	(7)	.0329	(8)	.0329
(9)	.0000	(10)	.0001	(11)	-.0011	(12)	-.0010
(13)	.0334						

0.brus1.4
0*** element node table temperature = 25.000 deg c

0*****

0	0	rg1	rg2	rg3	rg4	rg5	rg6	rg7
0	1	rg8	rg9	rg10	rg11	rg12	rg13	
0	2	r1	rg1	ca	cx	cy		
0	3	rg2	da	ce	cx	d1	d2	d7
0	4	r1	r2	rg3				
0	5	r2	rg4	ce				
0	6	rg5	cb	d1				
0	7	r4	rg6	d2				
0	8	rg7	cy	d5				
0	9	rg8	cd	d6				
0	10	rg9	cd	d4				
0	11	r3	rg10	d4				
0	12	rg12	rg11	d3				
0	13	r4	cb	d3				
1			rg13	d7				

1***** e ***** spice 2.Xx (vax11/780) *****

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voltage source currents

```

name      current
vse      3.320e-02
vsd      9.987e-04
    
```

total power dissipation 6.66e-03 watts
 0**** operating point information temperature = 25.000 deg c

0**** voltage-controlled current sources

```

0          qlvccs  qvccs
i-source  9.99e-04  1.00e-03
    
```

0**** diodes

```

0          d1      d2      d3      d4      d5      d6      d7
0model    dmod1    dmod2    dmod3    dmod3a  dmod4    dmod5    dmod6
id        3.32e-05  1.10e-03  9.98e-04 -9.99e-04 -6.58e-05  3.29e-05  9.66e-04
vd        .000    .000    .000    .000    .000    .000    .000
0**** transient analysis temperature = 25.000 deg c
    
```

time	v(0,1)	v(0,12)
0.000e+00	-6.660e-02	9.978e-04
1.000e-03	-1.984e-01	-4.507e-02
2.000e-03	-3.743e-01	-8.711e-02
3.000e-03	-4.755e-01	-9.746e-02
4.000e-03	-5.339e-01	-9.500e-02
5.000e-03	-5.688e-01	-8.861e-02
6.000e-03	-5.905e-01	-8.139e-02
7.000e-03	-6.046e-01	-7.439e-02
8.000e-03	-6.141e-01	-6.792e-02
9.000e-03	-6.209e-01	-6.203e-02
1.000e-02	-6.261e-01	-5.669e-02
1.100e-02	-6.807e-01	-2.729e-01
1.200e-02	-7.288e-01	-4.630e-01
1.300e-02	-7.435e-01	-5.829e-01
1.400e-02	-7.444e-01	-6.647e-01
1.500e-02	-7.403e-01	-7.239e-01
1.600e-02	-7.345e-01	-7.701e-01
1.700e-02	-6.770e-01	-6.008e-01
1.800e-02	-6.265e-01	-4.226e-01
1.900e-02	-6.102e-01	-3.191e-01
2.000e-02	-6.075e-01	-2.521e-01
2.100e-02	-6.102e-01	-2.055e-01

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2.200e-02	-6.144e-01	-1.705e-01
2.300e-02	-6.188e-01	-1.430e-01
2.400e-02	-6.229e-01	-1.209e-01
2.500e-02	-6.267e-01	-1.029e-01
2.600e-02	-6.301e-01	-8.818e-02
2.700e-02	-6.332e-01	-7.601e-02
2.800e-02	-6.360e-01	-6.590e-02
2.900e-02	-6.385e-01	-5.745e-02
3.000e-02	-6.408e-01	-5.026e-02
3.100e-02	-6.935e-01	-2.658e-01
3.200e-02	-7.390e-01	-4.524e-01
3.300e-02	-7.528e-01	-5.717e-01
3.400e-02	-7.535e-01	-6.546e-01
3.500e-02	-7.486e-01	-7.143e-01
3.600e-02	-7.422e-01	-7.610e-01
3.700e-02	-6.841e-01	-5.919e-01
3.800e-02	-6.331e-01	-4.142e-01
3.900e-02	-6.163e-01	-3.112e-01
4.000e-02	-6.132e-01	-2.447e-01
4.100e-02	-6.154e-01	-1.986e-01
4.200e-02	-6.192e-01	-1.639e-01
4.300e-02	-6.232e-01	-1.368e-01
4.400e-02	-6.270e-01	-1.152e-01
4.500e-02	-6.305e-01	-9.757e-02
4.600e-02	-6.336e-01	-8.321e-02
4.700e-02	-6.364e-01	-7.139e-02
4.800e-02	-6.390e-01	-6.160e-02
4.900e-02	-6.413e-01	-5.346e-02
5.000e-02	-6.433e-01	-4.656e-02

y
0*** transient analysis . . . temperature = 25.000-deg c

x	time	v(1,2)	v(12,5)	v(4,2)	v(9,8)
	0.000e+00	6.660e-02	-3.420e-02	0.000e+00	-3.289e-02
	1.000e-03	1.445e-01	-3.786e-02	-5.391e-02	-5.509e-02
	2.000e-03	2.549e-01	-5.265e-02	-1.193e-01	-9.716e-02
	3.000e-03	3.194e-01	-7.213e-02	-1.560e-01	-1.273e-01
	4.000e-03	3.557e-01	-9.242e-02	-1.781e-01	-1.496e-01
	5.000e-03	3.758e-01	-1.118e-01	-1.930e-01	-1.671e-01
	6.000e-03	3.864e-01	-1.297e-01	-2.041e-01	-1.816e-01
	7.000e-03	3.916e-01	-1.462e-01	-2.130e-01	-1.939e-01
	8.000e-03	3.937e-01	-1.613e-01	-2.205e-01	-2.048e-01
	9.000e-03	3.940e-01	-1.751e-01	-2.270e-01	-2.146e-01
	1.000e-02	3.933e-01	-1.877e-01	-2.327e-01	-2.236e-01
	1.100e-02	3.901e-01	-1.124e-01	-2.906e-01	-2.555e-01
	1.200e-02	3.816e-01	1.560e-02	-3.472e-01	-3.073e-01
	1.300e-02	3.723e-01	1.134e-01	-3.712e-01	-3.456e-01
	1.400e-02	3.641e-01	1.913e-01	-3.805e-01	-3.735e-01
	1.500e-02	3.576e-01	2.545e-01	-3.826e-01	-3.930e-01
	1.600e-02	3.527e-01	3.074e-01	-3.818e-01	-4.066e-01
	1.700e-02	3.515e-01	2.632e-01	-3.255e-01	-3.914e-01
	1.800e-02	3.566e-01	1.595e-01	-2.699e-01	-3.511e-01
	1.900e-02	3.631e-01	8.301e-02	-2.470e-01	-3.214e-01

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2.000e-02	3.692e-01	2.318e-02	-2.383e-01	-3.000e-01
2.100e-02	3.741e-01	-2.480e-02	-2.361e-01	-2.851e-01
2.200e-02	3.778e-01	-6.425e-02	-2.366e-01	-2.750e-01
2.300e-02	3.804e-01	-9.718e-02	-2.384e-01	-2.686e-01
2.400e-02	3.821e-01	-1.249e-01	-2.409e-01	-2.650e-01
2.500e-02	3.831e-01	-1.485e-01	-2.436e-01	-2.634e-01
2.600e-02	3.836e-01	-1.687e-01	-2.466e-01	-2.634e-01
2.700e-02	3.837e-01	-1.860e-01	-2.495e-01	-2.645e-01
2.800e-02	3.835e-01	-2.010e-01	-2.525e-01	-2.663e-01
2.900e-02	3.831e-01	-2.141e-01	-2.554e-01	-2.687e-01
3.000e-02	3.825e-01	-2.257e-01	-2.583e-01	-2.715e-01
3.100e-02	3.798e-01	-1.490e-01	-3.137e-01	-2.982e-01
3.200e-02	3.720e-01	-2.034e-02	-3.670e-01	-3.452e-01
3.300e-02	3.636e-01	7.890e-02	-3.892e-01	-3.795e-01
3.400e-02	3.562e-01	1.590e-01	-3.974e-01	-4.042e-01
3.500e-02	3.504e-01	2.243e-01	-3.983e-01	-4.209e-01
3.600e-02	3.461e-01	2.793e-01	-3.962e-01	-4.321e-01
3.700e-02	3.454e-01	2.370e-01	-3.387e-01	-4.146e-01
3.800e-02	3.511e-01	1.351e-01	-2.820e-01	-3.723e-01
3.900e-02	3.581e-01	6.029e-02	-2.582e-01	-3.408e-01
4.000e-02	3.646e-01	2.058e-03	-2.485e-01	-3.178e-01
4.100e-02	3.699e-01	-4.442e-02	-2.455e-01	-3.014e-01
4.200e-02	3.740e-01	-8.246e-02	-2.453e-01	-2.900e-01
4.300e-02	3.769e-01	-1.141e-01	-2.464e-01	-2.824e-01
4.400e-02	3.789e-01	-1.406e-01	-2.482e-01	-2.776e-01
4.500e-02	3.802e-01	-1.630e-01	-2.503e-01	-2.750e-01
4.600e-02	3.809e-01	-1.871e-01	-2.527e-01	-2.741e-01
4.700e-02	3.812e-01	-1.984e-01	-2.552e-01	-2.743e-01
4.800e-02	3.812e-01	-2.125e-01	-2.577e-01	-2.754e-01
4.900e-02	3.810e-01	-2.247e-01	-2.602e-01	-2.771e-01
5.000e-02	3.807e-01	-2.355e-01	-2.627e-01	-2.792e-01

Y
0**** transient analysis temperature = 25.000 deg.c

X	time	v(3,2)	v(7,2)
	0.000e+00	3.320e-02	3.289e-02
	1.000e-03	3.146e-02	1.394e-02
	2.000e-03	2.505e-02	-1.232e-02
	3.000e-03	1.869e-02	-2.153e-02
	4.000e-03	1.432e-02	-2.296e-02
	5.000e-03	1.205e-02	-2.141e-02
	6.000e-03	1.132e-02	-1.876e-02
	7.000e-03	1.156e-02	-1.574e-02
	8.000e-03	1.236e-02	-1.264e-02
	9.000e-03	1.344e-02	-9.605e-03
	1.000e-02	1.466e-02	-6.685e-03
	1.100e-02	4.005e-02	-1.957e-02
	1.200e-02	6.506e-02	-2.734e-02
	1.300e-02	7.274e-02	-1.640e-02
	1.400e-02	7.325e-02	-3.821e-04
	1.500e-02	7.099e-02	1.498e-02
	1.600e-02	6.799e-02	2.787e-02
	1.700e-02	4.055e-02	5.291e-02

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1.800e-02	1.375e-02	7.045e-02
1.900e-02	4.916e-03	6.682e-02
2.000e-02	3.415e-03	5.645e-02
2.100e-02	4.772e-03	4.542e-02
2.200e-02	6.923e-03	3.607e-02
2.300e-02	9.167e-03	2.881e-02
2.400e-02	1.128e-02	2.344e-02
2.500e-02	1.321e-02	1.963e-02
2.600e-02	1.495e-02	1.704e-02
2.700e-02	1.652e-02	1.540e-02
2.800e-02	1.794e-02	1.448e-02
2.900e-02	1.922e-02	1.411e-02
3.000e-02	2.039e-02	1.411e-02
3.100e-02	4.557e-02	-1.161e-03
3.200e-02	6.972e-02	-1.032e-02
3.300e-02	7.720e-02	-1.432e-03
3.400e-02	7.775e-02	1.260e-02
3.500e-02	7.530e-02	2.651e-02
3.600e-02	7.206e-02	3.825e-02
3.700e-02	4.436e-02	6.226e-02
3.800e-02	1.731e-02	7.894e-02
3.900e-02	8.231e-03	7.456e-02
4.000e-02	6.499e-03	6.351e-02
4.100e-02	7.640e-03	5.188e-02
4.200e-02	9.590e-03	4.200e-02
4.300e-02	1.165e-02	3.425e-02
4.400e-02	1.359e-02	2.844e-02
4.500e-02	1.535e-02	2.423e-02
4.600e-02	1.695e-02	2.128e-02
4.700e-02	1.838e-02	1.931e-02
4.800e-02	1.967e-02	1.810e-02
4.900e-02	2.084e-02	1.745e-02
5.000e-02	2.190e-02	1.720e-02

Y
0**** transient analysis temperature = 25.000 deg c

X	time	v(3,5)	v(12,11)	v(9,10)	v(7,8)
	0.000e+00	1.768e-06	7.351e-05	-9.558e-05	2.001e-06
	1.000e-03	2.434e-03	8.030e-05	-9.999e-05	1.275e-02
	2.000e-03	4.607e-03	8.649e-05	-1.040e-04	9.842e-03
	3.000e-03	-5.134e-03	8.802e-05	-1.050e-04	7.184e-03
	4.000e-03	5.010e-03	8.766e-05	-1.048e-04	5.531e-03
	5.000e-03	4.685e-03	8.671e-05	-1.042e-04	4.501e-03
	6.000e-03	4.316e-03	8.565e-05	-1.035e-04	3.808e-03
	7.000e-03	3.958e-03	8.462e-05	-1.028e-04	3.333e-03
	8.000e-03	3.625e-03	8.367e-05	-1.022e-04	2.978e-03
	9.000e-03	3.322e-03	8.280e-05	-1.016e-04	2.704e-03
	1.000e-02	3.046e-03	8.201e-05	-1.011e-04	2.475e-03
	1.100e-02	-5.463e-02	1.139e-04	-1.218e-04	1.553e-02
	1.200e-02	-3.512e-02	1.418e-04	-1.400e-04	1.255e-02
	1.300e-02	-2.557e-02	1.595e-04	-1.515e-04	9.192e-03
	1.400e-02	-1.976e-02	1.716e-04	-1.593e-04	6.593e-03
	1.500e-02	-1.586e-02	1.803e-04	-1.650e-04	4.593e-03

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1.600e-02	-1.294e-02	1.871e-04	-1.694e-04	3.023e-03
1.700e-02	2.842e-02	1.621e-04	-1.532e-04	-1.298e-02
1.800e-02	2.061e-02	1.359e-04	-1.361e-04	-1.072e-02
1.900e-02	1.588e-02	1.207e-04	-1.262e-04	-7.572e-03
2.000e-02	1.274e-02	1.108e-04	-1.198e-04	-5.263e-03
2.100e-02	1.050e-02	1.039e-04	-1.153e-04	-3.589e-03
2.200e-02	8.788e-03	9.877e-05	-1.120e-04	-2.330e-03
2.300e-02	7.426e-03	9.472e-05	-1.094e-04	-1.398e-03
2.400e-02	6.321e-03	9.147e-05	-1.072e-04	-6.982e-04
2.500e-02	5.415e-03	8.882e-05	-1.055e-04	-1.844e-04
2.600e-02	4.666e-03	8.665e-05	-1.041e-04	1.939e-04
2.700e-02	4.043e-03	8.486e-05	-1.030e-04	4.640e-04
2.800e-02	3.523e-03	8.337e-05	-1.020e-04	6.544e-04
2.900e-02	3.086e-03	8.212e-05	-1.012e-04	7.817e-04
3.000e-02	2.714e-03	8.106e-05	-1.005e-04	8.655e-04
3.100e-02	-5.554e-02	1.128e-04	-1.211e-04	1.427e-02
3.200e-02	-3.600e-02	1.403e-04	-1.390e-04	1.150e-02
3.300e-02	-2.642e-02	1.579e-04	-1.504e-04	8.277e-03
3.400e-02	-2.046e-02	1.701e-04	-1.583e-04	5.766e-03
3.500e-02	-1.648e-02	1.789e-04	-1.640e-04	3.850e-03
3.600e-02	-1.350e-02	1.857e-04	-1.685e-04	2.345e-03
3.700e-02	2.805e-02	1.609e-04	-1.523e-04	-1.367e-02
3.800e-02	2.023e-02	1.347e-04	-1.353e-04	-1.133e-02
3.900e-02	1.551e-02	1.195e-04	-1.255e-04	-8.111e-03
4.000e-02	1.238e-02	1.097e-04	-1.191e-04	-5.740e-03
4.100e-02	1.016e-02	1.029e-04	-1.147e-04	-4.014e-03
4.200e-02	8.465e-03	9.781e-05	-1.114e-04	-2.711e-03
4.300e-02	7.121e-03	9.382e-05	-1.088e-04	-1.742e-03
4.400e-02	6.033e-03	9.062e-05	-1.067e-04	-1.010e-03
4.500e-02	5.144e-03	8.803e-05	-1.050e-04	-4.680e-04
4.600e-02	4.412e-03	8.592e-05	-1.036e-04	-6.452e-05
4.700e-02	3.806e-03	8.418e-05	-1.025e-04	2.279e-04
4.800e-02	3.302e-03	8.274e-05	-1.016e-04	4.383e-04
4.900e-02	2.880e-03	8.154e-05	-1.008e-04	5.837e-04
5.000e-02	2.522e-03	8.052e-05	-1.001e-04	6.839e-04

0**** transient analysis temperature = 25.000 deg c

x	time	v(13,3)	v(3,6)	v(7,6)
	0.000e+00	1.697e-04	3.028e-04	-6.953e-06
	1.000e-03	1.584e-04	1.273e-02	-4.799e-03
	2.000e-03	1.457e-04	2.699e-02	-1.038e-02
	3.000e-03	1.400e-04	2.903e-02	-1.119e-02
	4.000e-03	1.372e-04	2.692e-02	-1.035e-02
	5.000e-03	1.355e-04	2.419e-02	-9.273e-03
	6.000e-03	1.340e-04	2.177e-02	-8.318e-03
	7.000e-03	1.328e-04	1.977e-02	-7.532e-03
	8.000e-03	1.316e-04	1.811e-02	-6.885e-03
	9.000e-03	1.305e-04	1.671e-02	-6.336e-03
	1.000e-02	1.295e-04	1.549e-02	-5.857e-03
	1.100e-02	1.103e-04	4.290e-02	-1.672e-02
	1.200e-02	9.233e-05	6.615e-02	-2.624e-02
	1.300e-02	8.712e-05	6.385e-02	-2.528e-02

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1.400e-02	8.713e-05	5.287e-02	-2.076e-02
1.500e-02	8.916e-05	4.033e-02	-1.567e-02
1.600e-02	9.169e-05	2.898e-02	-1.114e-02
1.700e-02	1.129e-04	-8.842e-03	3.519e-03
1.800e-02	1.333e-04	-4.112e-02	1.558e-02
1.900e-02	1.396e-04	-4.492e-02	1.698e-02
2.000e-02	1.402e-04	-3.844e-02	1.459e-02
2.100e-02	1.387e-04	-2.940e-02	1.124e-02
2.200e-02	1.366e-04	-2.104e-02	8.111e-03
2.300e-02	1.347e-04	-1.413e-02	5.511e-03
2.400e-02	1.329e-04	-8.706e-03	3.456e-03
2.500e-02	1.313e-04	-4.547e-03	1.872e-03
2.600e-02	1.299e-04	-1.415e-03	6.755e-04
2.700e-02	1.287e-04	9.052e-04	-2.135e-04
2.800e-02	1.277e-04	2.592e-03	-8.611e-04
2.900e-02	1.267e-04	3.789e-03	-1.321e-03
3.000e-02	1.259e-04	4.631e-03	-1.645e-03
3.100e-02	1.068e-04	3.371e-02	-1.303e-02
3.200e-02	8.939e-05	5.742e-02	-2.262e-02
3.300e-02	8.434e-05	5.642e-02	-2.221e-02
3.400e-02	8.433e-05	4.684e-02	-1.830e-02
3.500e-02	8.649e-05	3.519e-02	-1.361e-02
3.600e-02	8.920e-05	2.446e-02	-9.351e-03
3.700e-02	1.106e-04	-1.286e-02	5.044e-03
3.800e-02	1.313e-04	-4.472e-02	1.691e-02
3.900e-02	1.377e-04	-4.815e-02	1.817e-02
4.000e-02	1.384e-04	-4.135e-02	1.567e-02
4.100e-02	1.370e-04	-3.202e-02	1.222e-02
4.200e-02	1.351e-04	-2.341e-02	9.001e-03
4.300e-02	1.332e-04	-1.628e-02	6.323e-03
4.400e-02	1.315e-04	-1.066e-02	4.197e-03
4.500e-02	1.301e-04	-6.324e-03	2.551e-03
4.600e-02	1.288e-04	-3.037e-03	1.297e-03
4.700e-02	1.277e-04	-5.770e-04	3.557e-04
4.800e-02	1.267e-04	1.236e-03	-3.391e-04
4.900e-02	1.258e-04	2.546e-03	-8.423e-04
5.000e-02	-1.250e-04	3.492e-03	-1.206e-03

y
0**** transient analysis temperature = 25.000 deg c)

x	time	v(3,1)	v(3,4)	v(11,10)	v(6,13)
	0.000e+00	-3.340e-02	3.320e-02	-1.167e-03	-4.725e-04
	1.000e-03	-1.131e-01	8.537e-02	4.489e-02	-1.289e-02
	2.000e-03	-2.299e-01	1.444e-01	8.692e-02	-2.713e-02
	3.000e-03	-3.008e-01	1.747e-01	9.726e-02	-2.917e-02
	4.000e-03	-3.414e-01	1.924e-01	9.481e-02	-2.706e-02
	5.000e-03	-3.637e-01	2.051e-01	8.842e-02	-2.433e-02
	6.000e-03	-3.751e-01	2.155e-01	8.120e-02	-2.190e-02
	7.000e-03	-3.800e-01	2.246e-01	7.420e-02	-1.990e-02
	8.000e-03	-3.813e-01	2.328e-01	6.773e-02	-1.825e-02
	9.000e-03	-3.805e-01	2.404e-01	6.184e-02	-1.684e-02
	1.000e-02	-3.787e-01	2.474e-01	5.650e-02	-1.562e-02
	1.100e-02	-3.500e-01	3.307e-01	2.727e-01	-4.301e-02

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1.200e-02	-3.165e-01	4.123e-01	4.627e-01	-6.625e-02
1.300e-02	-2.996e-01	4.439e-01	5.826e-01	-6.394e-02
1.400e-02	-2.909e-01	4.537e-01	6.644e-01	-5.296e-02
1.500e-02	-2.867e-01	4.536e-01	7.236e-01	-4.042e-02
1.600e-02	-2.847e-01	4.498e-01	7.697e-01	-2.908e-02
1.700e-02	-3.109e-01	3.660e-01	6.004e-01	8.729e-03
1.800e-02	-3.428e-01	2.836e-01	4.223e-01	4.098e-02
1.900e-02	-3.582e-01	2.519e-01	3.188e-01	4.478e-02
2.000e-02	-3.658e-01	2.417e-01	2.519e-01	3.830e-02
2.100e-02	-3.694e-01	2.408e-01	2.053e-01	2.926e-02
2.200e-02	-3.709e-01	2.435e-01	1.703e-01	2.090e-02
2.300e-02	-3.712e-01	2.476e-01	1.428e-01	1.400e-02
2.400e-02	-3.708e-01	2.521e-01	1.207e-01	8.574e-03
2.500e-02	-3.699e-01	2.568e-01	1.027e-01	4.415e-03
2.600e-02	-3.686e-01	2.615e-01	8.799e-02	1.285e-03
2.700e-02	-3.671e-01	2.661e-01	7.582e-02	-1.034e-03
2.800e-02	-3.655e-01	2.704e-01	6.572e-02	-2.720e-03
2.900e-02	-3.639e-01	2.746e-01	5.727e-02	-3.916e-03
3.000e-02	-3.621e-01	2.786e-01	5.008e-02	-4.757e-03
3.100e-02	-3.342e-01	3.592e-01	2.656e-01	-3.382e-02
3.200e-02	-3.023e-01	4.367e-01	4.521e-01	-5.751e-02
3.300e-02	-2.864e-01	4.664e-01	5.714e-01	-5.650e-02
3.400e-02	-2.784e-01	4.751e-01	6.543e-01	-4.693e-02
3.500e-02	-2.751e-01	4.736e-01	7.140e-01	-3.527e-02
3.600e-02	-2.740e-01	4.682e-01	7.607e-01	-2.455e-02
3.700e-02	-3.011e-01	3.830e-01	5.916e-01	1.275e-02
3.800e-02	-3.338e-01	2.993e-01	4.140e-01	4.459e-02
3.900e-02	-3.499e-01	2.664e-01	3.109e-01	4.802e-02
4.000e-02	-3.581e-01	2.550e-01	2.445e-01	4.121e-02
4.100e-02	-3.623e-01	2.531e-01	1.983e-01	3.189e-02
4.200e-02	-3.644e-01	2.549e-01	1.637e-01	2.327e-02
4.300e-02	-3.652e-01	2.580e-01	1.366e-01	1.615e-02
4.400e-02	-3.653e-01	2.618e-01	1.150e-01	1.053e-02
4.500e-02	-3.648e-01	2.657e-01	9.738e-02	6.194e-03
4.600e-02	-3.640e-01	2.697e-01	8.302e-02	2.908e-03
4.700e-02	-3.628e-01	2.736e-01	7.120e-02	4.493e-04
4.800e-02	-3.616e-01	2.774e-01	6.142e-02	-1.362e-03
4.900e-02	-3.602e-01	2.811e-01	5.328e-02	-2.672e-03
5.000e-02	-3.588e-01	2.846e-01	4.638e-02	-3.617e-03

y
0**** transient analysis temperature = 25.000 deg c

time	v(1)	v(2)	v(3)	v(4)
0.000e+00	6.660e-02	0.000e+00	3.320e-02	0.000e+00
1.000e-03	1.984e-01	5.391e-02	8.537e-02	0.000e+00
2.000e-03	3.743e-01	1.193e-01	1.444e-01	0.000e+00
3.000e-03	4.755e-01	1.560e-01	1.747e-01	0.000e+00
4.000e-03	5.339e-01	1.781e-01	1.924e-01	0.000e+00
5.000e-03	5.688e-01	1.930e-01	2.051e-01	0.000e+00
6.000e-03	5.905e-01	2.041e-01	2.155e-01	0.000e+00
7.000e-03	6.046e-01	2.130e-01	2.246e-01	0.000e+00
8.000e-03	6.141e-01	2.205e-01	2.328e-01	0.000e+00
9.000e-03	6.209e-01	2.270e-01	2.404e-01	0.000e+00

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1.000e-02	6.261e-01	2.327e-01	2.474e-01	0.000e+00
1.100e-02	6.807e-01	2.906e-01	3.307e-01	0.000e+00
1.200e-02	7.288e-01	3.472e-01	4.123e-01	0.000e+00
1.300e-02	7.435e-01	3.712e-01	4.439e-01	0.000e+00
1.400e-02	7.446e-01	3.805e-01	4.537e-01	0.000e+00
1.500e-02	7.403e-01	3.826e-01	4.536e-01	0.000e+00
1.600e-02	7.345e-01	3.818e-01	4.498e-01	0.000e+00
1.700e-02	6.770e-01	3.255e-01	3.660e-01	0.000e+00
1.800e-02	6.265e-01	2.699e-01	2.836e-01	0.000e+00
1.900e-02	6.102e-01	2.470e-01	2.519e-01	0.000e+00
2.000e-02	6.075e-01	2.383e-01	2.417e-01	0.000e+00
2.100e-02	6.102e-01	2.361e-01	2.408e-01	0.000e+00
2.200e-02	6.144e-01	2.366e-01	2.435e-01	0.000e+00
2.300e-02	6.188e-01	2.384e-01	2.476e-01	0.000e+00
2.400e-02	6.229e-01	2.409e-01	2.521e-01	0.000e+00
2.500e-02	6.267e-01	2.436e-01	2.568e-01	0.000e+00
2.600e-02	6.301e-01	2.466e-01	2.615e-01	0.000e+00
2.700e-02	6.332e-01	2.495e-01	2.661e-01	0.000e+00
2.800e-02	6.360e-01	2.525e-01	2.704e-01	0.000e+00
2.900e-02	6.385e-01	2.554e-01	2.746e-01	0.000e+00
3.000e-02	6.408e-01	2.583e-01	2.786e-01	0.000e+00
3.100e-02	6.435e-01	3.137e-01	3.592e-01	0.000e+00
3.200e-02	7.390e-01	3.670e-01	4.367e-01	0.000e+00
3.300e-02	7.528e-01	3.892e-01	4.664e-01	0.000e+00
3.400e-02	7.535e-01	3.974e-01	4.751e-01	0.000e+00
3.500e-02	7.486e-01	3.983e-01	4.736e-01	0.000e+00
3.600e-02	7.422e-01	3.962e-01	4.682e-01	0.000e+00
3.700e-02	6.841e-01	3.387e-01	3.830e-01	0.000e+00
3.800e-02	6.331e-01	2.820e-01	2.993e-01	0.000e+00
3.900e-02	6.163e-01	2.582e-01	2.664e-01	0.000e+00
4.000e-02	6.132e-01	2.485e-01	2.550e-01	0.000e+00
4.100e-02	6.154e-01	2.455e-01	2.531e-01	0.000e+00
4.200e-02	6.192e-01	2.453e-01	2.549e-01	0.000e+00
4.300e-02	6.232e-01	2.464e-01	2.580e-01	0.000e+00
4.400e-02	6.270e-01	2.482e-01	2.618e-01	0.000e+00
4.500e-02	6.305e-01	2.503e-01	2.657e-01	0.000e+00
4.600e-02	6.336e-01	2.527e-01	2.697e-01	0.000e+00
4.700e-02	6.364e-01	2.552e-01	2.736e-01	0.000e+00
4.800e-02	6.390e-01	2.577e-01	2.774e-01	0.000e+00
4.900e-02	6.413e-01	2.602e-01	2.811e-01	0.000e+00
5.000e-02	6.433e-01	2.627e-01	2.846e-01	0.000e+00

Y
0**** transient analysis temperature = 25.000 deg c

x	time	v(5)	v(6)	v(7)	v(8)
	0.000e+00	3.320e-02	3.290e-02	3.289e-02	3.289e-02
	1.000e-03	8.294e-02	7.264e-02	6.784e-02	5.509e-02
	2.000e-03	1.398e-01	1.174e-01	1.070e-01	9.716e-02
	3.000e-03	1.696e-01	1.457e-01	1.345e-01	1.273e-01
	4.000e-03	1.874e-01	1.655e-01	1.552e-01	1.496e-01
	5.000e-03	2.004e-01	1.809e-01	1.716e-01	1.671e-01
	6.000e-03	2.111e-01	1.937e-01	1.854e-01	1.816e-01
	7.000e-03	2.206e-01	2.048e-01	1.973e-01	1.939e-01

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8.000e-03	2.292e-01	2.147e-01	2.078e-01	2.048e-01
9.000e-03	2.371e-01	2.237e-01	2.173e-01	2.146e-01
1.000e-02	2.443e-01	2.319e-01	2.260e-01	2.236e-01
1.100e-02	3.853e-01	2.877e-01	2.710e-01	2.555e-01
1.200e-02	4.474e-01	3.461e-01	3.199e-01	3.073e-01
1.300e-02	4.695e-01	3.801e-01	3.548e-01	3.456e-01
1.400e-02	4.735e-01	4.008e-01	3.801e-01	3.735e-01
1.500e-02	4.695e-01	4.133e-01	3.976e-01	3.930e-01
1.600e-02	4.627e-01	4.209e-01	4.096e-01	4.066e-01
1.700e-02	3.376e-01	3.749e-01	3.784e-01	3.914e-01
1.800e-02	2.630e-01	3.248e-01	3.403e-01	3.511e-01
1.900e-02	2.360e-01	2.968e-01	3.138e-01	3.214e-01
2.000e-02	2.290e-01	2.801e-01	2.947e-01	3.000e-01
2.100e-02	2.303e-01	2.702e-01	2.815e-01	2.851e-01
2.200e-02	2.347e-01	2.646e-01	2.727e-01	2.750e-01
2.300e-02	2.402e-01	2.617e-01	2.672e-01	2.686e-01
2.400e-02	2.458e-01	2.608e-01	2.643e-01	2.650e-01
2.500e-02	2.514e-01	2.614e-01	2.633e-01	2.634e-01
2.600e-02	2.568e-01	2.629e-01	2.636e-01	2.634e-01
2.700e-02	2.620e-01	2.652e-01	2.649e-01	2.645e-01
2.800e-02	2.669e-01	2.679e-01	2.670e-01	2.663e-01
2.900e-02	2.716e-01	2.709e-01	2.695e-01	2.687e-01
3.000e-02	2.759e-01	2.740e-01	2.724e-01	2.715e-01
3.100e-02	4.148e-01	3.255e-01	3.125e-01	2.982e-01
3.200e-02	4.727e-01	3.793e-01	3.567e-01	3.452e-01
3.300e-02	4.928e-01	4.100e-01	3.878e-01	3.795e-01
3.400e-02	4.956e-01	4.293e-01	4.100e-01	4.042e-01
3.500e-02	4.900e-01	4.384e-01	4.248e-01	4.209e-01
3.600e-02	4.817e-01	4.438e-01	4.344e-01	4.321e-01
3.700e-02	3.550e-01	3.959e-01	4.009e-01	4.146e-01
3.800e-02	2.791e-01	3.441e-01	3.610e-01	3.723e-01
3.900e-02	2.509e-01	3.145e-01	3.327e-01	3.408e-01
4.000e-02	2.426e-01	2.964e-01	3.120e-01	3.178e-01
4.100e-02	2.430e-01	2.851e-01	2.974e-01	3.014e-01
4.200e-02	2.464e-01	2.783e-01	2.873e-01	2.900e-01
4.300e-02	2.509e-01	2.743e-01	2.806e-01	2.824e-01
4.400e-02	2.557e-01	2.724e-01	2.766e-01	2.776e-01
4.500e-02	2.606e-01	2.720e-01	2.746e-01	2.750e-01
4.600e-02	2.653e-01	2.727e-01	2.740e-01	2.741e-01
4.700e-02	2.698e-01	2.742e-01	2.745e-01	2.743e-01
4.800e-02	2.741e-01	2.762e-01	2.758e-01	2.754e-01
4.900e-02	2.782e-01	2.785e-01	2.777e-01	2.771e-01
5.000e-02	2.820e-01	2.811e-01	2.799e-01	2.792e-01

y
0*** transient analysis temperature = 25.000 deg c

x	time	v(9)	v(10)	v(11)	v(12)	v(13)
	0.000e+00	0.000e+00	9.558e-05	-1.071e-03	-9.978e-04	3.337e-02
	1.000e-03	0.000e+00	9.999e-05	4.499e-02	4.507e-02	8.553e-02
	2.000e-03	0.000e+00	1.040e-04	8.703e-02	8.711e-02	1.445e-01
	3.000e-03	0.000e+00	1.050e-04	9.737e-02	9.746e-02	1.749e-01
	4.000e-03	0.000e+00	1.048e-04	9.492e-02	9.500e-02	1.926e-01
	5.000e-03	0.000e+00	1.042e-04	8.853e-02	8.861e-02	2.052e-01

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6.000e-03	0.000e+00	1.035e-04	8.131e-02	8.139e-02	2.156e-01
7.000e-03	0.000e+00	1.028e-04	7.431e-02	7.439e-02	2.247e-01
8.000e-03	0.000e+00	1.022e-04	6.783e-02	6.792e-02	2.330e-01
9.000e-03	0.000e+00	1.016e-04	6.194e-02	6.203e-02	2.405e-01
1.000e-02	0.000e+00	1.011e-04	5.661e-02	5.669e-02	2.475e-01
1.100e-02	0.000e+00	1.218e-04	2.728e-01	2.729e-01	3.308e-01
1.200e-02	0.000e+00	1.400e-04	4.628e-01	4.630e-01	4.124e-01
1.300e-02	0.000e+00	1.515e-04	5.827e-01	5.829e-01	4.440e-01
1.400e-02	0.000e+00	1.593e-04	6.646e-01	6.647e-01	4.538e-01
1.500e-02	0.000e+00	1.650e-04	7.238e-01	7.239e-01	4.537e-01
1.600e-02	0.000e+00	1.694e-04	7.699e-01	7.701e-01	4.499e-01
1.700e-02	0.000e+00	1.532e-04	6.006e-01	6.008e-01	3.661e-01
1.800e-02	0.000e+00	1.361e-04	4.225e-01	4.226e-01	2.838e-01
1.900e-02	0.000e+00	1.262e-04	3.189e-01	3.191e-01	2.521e-01
2.000e-02	0.000e+00	1.198e-04	2.520e-01	2.521e-01	2.418e-01
2.100e-02	0.000e+00	1.153e-04	2.054e-01	2.055e-01	2.410e-01
2.200e-02	0.000e+00	1.120e-04	1.704e-01	1.705e-01	2.437e-01
2.300e-02	0.000e+00	1.094e-04	1.429e-01	1.430e-01	2.477e-01
2.400e-02	0.000e+00	1.072e-04	1.208e-01	1.209e-01	2.523e-01
2.500e-02	0.000e+00	1.055e-04	1.028e-01	1.029e-01	2.570e-01
2.600e-02	0.000e+00	1.041e-04	8.810e-02	8.818e-02	2.616e-01
2.700e-02	0.000e+00	1.030e-04	7.593e-02	7.601e-02	2.662e-01
2.800e-02	0.000e+00	1.020e-04	6.582e-02	6.590e-02	2.706e-01
2.900e-02	0.000e+00	1.012e-04	5.737e-02	5.745e-02	2.748e-01
3.000e-02	0.000e+00	1.005e-04	5.018e-02	5.026e-02	2.788e-01
3.100e-02	0.000e+00	1.211e-04	2.657e-01	2.658e-01	3.593e-01
3.200e-02	0.000e+00	1.390e-04	4.522e-01	4.524e-01	4.368e-01
3.300e-02	0.000e+00	1.504e-04	5.716e-01	5.717e-01	4.665e-01
3.400e-02	0.000e+00	1.583e-04	6.544e-01	6.546e-01	4.752e-01
3.500e-02	0.000e+00	1.640e-04	7.141e-01	7.143e-01	4.737e-01
3.600e-02	0.000e+00	1.685e-04	7.609e-01	7.610e-01	4.683e-01
3.700e-02	0.000e+00	1.523e-04	5.918e-01	5.919e-01	3.831e-01
3.800e-02	0.000e+00	1.353e-04	4.141e-01	4.142e-01	2.995e-01
3.900e-02	0.000e+00	1.255e-04	3.110e-01	3.112e-01	2.665e-01
4.000e-02	0.000e+00	1.191e-04	2.446e-01	2.447e-01	2.552e-01
4.100e-02	0.000e+00	1.147e-04	1.984e-01	1.986e-01	2.533e-01
4.200e-02	0.000e+00	1.114e-04	1.638e-01	1.639e-01	2.550e-01
4.300e-02	0.000e+00	1.088e-04	1.367e-01	1.368e-01	2.582e-01
4.400e-02	0.000e+00	1.067e-04	1.151e-01	1.152e-01	2.619e-01
4.500e-02	0.000e+00	1.050e-04	9.749e-02	9.757e-02	2.658e-01
4.600e-02	0.000e+00	1.036e-04	8.312e-02	8.321e-02	2.698e-01
4.700e-02	0.000e+00	1.025e-04	7.130e-02	7.139e-02	2.737e-01
4.800e-02	0.000e+00	1.016e-04	6.152e-02	6.160e-02	2.775e-01
4.900e-02	0.000e+00	1.008e-04	5.338e-02	5.346e-02	2.812e-01
5.000e-02	0.000e+00	1.001e-04	4.648e-02	4.656e-02	2.847e-01

y 0**** transient analysis temperature = 25.000 deg c

x time v(3,2) Plot 3

x	0.000e+00	2.000e-02	4.000e-02	6.000e-02	8.000e-02
0.000e+00	3.320e-02.	.	*	.	.
1.000e-03	3.146e-02.	.	*	.	.
2.000e-03	2.505e-02.	.	*	.	.

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***** spice 2.Rx (var1/780) *****
File 2
0,brus1,4a
**** transient analysis          Temperature = 25.000 deg c
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x	time	v(3,2)	0.000e+00	2.000e-02	4.000e-02	6.000e-02	8.000e-02
	0.000e+00	3.320e-02					
	1.000e-03	3.066e-02					
	2.000e-03	2.214e-02					
	3.000e-03	1.467e-02					
	4.000e-03	1.025e-02					
	5.000e-03	8.474e-03					
	6.000e-03	8.379e-03					
	7.000e-03	9.714e-03					
	8.000e-03	1.053e-02					
	9.000e-03	1.704e-02					
	1.000e-02	1.360e-02					
	1.100e-02	3.591e-02					
	1.200e-02	5.304e-02					
	1.300e-02	5.527e-02					
	1.400e-02	5.316e-02					
	1.500e-02	5.029e-02					
	1.600e-02	4.772e-02					
	1.700e-02	2.465e-02					
	1.800e-02	7.227e-03					
	1.900e-02	5.306e-03					
	2.000e-02	7.713e-03					
	2.100e-02	1.091e-02					
	2.200e-02	1.373e-02					
	2.300e-02	1.609e-02					
	2.400e-02	1.805e-02					
	2.500e-02	1.969e-02					
	2.600e-02	2.109e-02					
	2.700e-02	2.210e-02					
	2.800e-02	2.335e-02					
	2.900e-02	2.429e-02					
	3.000e-02	2.511e-02					
	3.100e-02	4.647e-02					
	3.200e-02	6.289e-02					
	3.300e-02	6.438e-02					
	3.400e-02	6.156e-02					
	3.500e-02	5.803e-02					
	3.600e-02	5.481e-02					
	3.700e-02	3.121e-02					
	3.800e-02	1.390e-02					
	3.900e-02	1.091e-02					
	4.000e-02	1.283e-02					
	4.100e-02	1.557e-02					
	4.200e-02	1.892e-02					
	4.300e-02	2.003e-02					
	4.400e-02	2.167e-02					
	4.500e-02	2.303e-02					
	4.600e-02	2.416e-02					
	4.700e-02	2.513e-02					
	4.800e-02	2.596e-02					
	4.900e-02	2.669e-02					
	5.000e-02	2.733e-02					

END

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FIN