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L'ÉNERGIE ATOMIQUE
DU CANADA LIMITÉE

MAKSIMA-CHEMIST
A PROGRAM FOR MASS ACTION KINETICS SIMULATION
BY AUTOMATIC CHEMICAL EQUATION MANIPULATION AND
INTEGRATION USING STIFF TECHNIQUES

MAKSIMA-CHEMIST
Programme de simulation cinétique pour actions de masse par
la manipulation automatique d'équations chimiques et par leur
intégration au moyen de techniques "rigides"

M.B. CARVER, D.V. HANLEY and K.R. CHAPLIN

Chalk River Nuclear Laboratories

Laboratoires nucléaires de Chalk River

Chalk River, Ontario

February 1979 février

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Résumé

MAKSIMA-CHEMIST a été écrit pour remplacer le programme WR20, lequel a été employé pendant quelque temps à Chalk River pour calculer la cinétique des réactions chimiques simultanées. Les équations différentielles ordinaires qui sont automatiquement dérivées des équations chimiques susmentionnées sont difficiles à intégrer car elles sont connectées d'une façon fortement non-linéaire et elles comportent fréquemment une vaste gamme dans la grandeur des taux de réaction. Elles forment une série d'équations différentielles classiques "rigides" ne pouvant être efficacement intégrées que par des techniques avancées récemment développées.

Ces techniques permettent à MAKSIMA-CHEMIST d'effectuer en quelques secondes des calculs qui nécessitent une nuit entière d'opérations sur WR20, ce qui augmente considérablement le potentiel des calculs cinétiques.

Le nouveau programme a également ce qu'il faut pour les réactions chimiques d'ordre élevé et il a un stockage dynamique et une caractéristique de décision. Cela lui permet d'accepter n'importe quel nombre de réactions et d'espèces chimiques et de choisir un plan d'intégration qui fonctionnera de façon très efficace dans la mémoire disponible. Des techniques faisant appel à des matrices éparses sont employées lorsque la structure et la dimension de la série d'équations le permet. Finalement, un certain nombre d'options post-analyse sont disponibles, y compris une imprimante, des points Calcomp de réponse transitoire d'espèces sélectionnées et une représentation graphique de la matrice de réaction.

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ABSTRACT

MAKSIMA-CHEMIST was written to replace the program WR20, which has been used for some time at CRNL*to compute the kinetics of simultaneous chemical reactions. The ordinary differential equations, which are automatically derived from the stated chemical equations, are difficult to integrate, as they are coupled in a highly nonlinear manner, and frequently involve a large range in the magnitude of the reaction rates. They form a classic 'stiff' differential equation set which can be integrated efficiently only by recently developed advanced techniques.

These techniques enable MAKSIMA-CHEMIST to complete, within a few seconds, calculations which require an overnight run on WR20, thus greatly expanding the potential of kinetics computation.

The new program also contains provision for higher order chemical reactions, and has a dynamic storage and decision feature. This permits it to accept any number of chemical reactions and species, and choose an integration scheme which will perform most efficiently within the available memory. Sparse matrix techniques are used when the size and structure of the equation set is suitable. Finally, a number of post-analysis options are available, including printer and Calcomp plots of transient response of selected species, and graphical representation of the reaction matrix.

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1. INTRODUCTION

1.1 Simplified Mass Action Kinetics

Consider the chemical equations



Reaction (1) removes A^- and BC from the system to form AB and C^- at a rate

$$R_1 = k_1 [A^-] [BC] \quad (3)$$

where $[]$ denotes concentration. Thus the total net rate of formation of AB from reactions 1 and 2 is

$$\frac{d}{dt}[AB] = k_1 [A^-] [BC] - k_2 [AB]^2 \quad (4)$$

further reactions involving AB as a reagent or product will generate further negative or positive terms respectively on the right-hand side of equation (4).

Thus the instantaneous concentration may be written

$$[A] = [AB]_0 + \int \left(\frac{d}{dt} [AB] \right) dt \quad (5)$$

and similar equations may be written for the other four species.

1.2 Integration

Current values for all species may then be obtained for any time by integrating the resulting five equations. The expressions for the derivatives (4) are nonlinear, thus the integration must be done numerically, and with an accurate technique, as the nonlinearity will quickly amplify any small errors. A further difficulty is

that in typical reaction sets, the individual reaction rates may differ by several orders of magnitude. This is the classical stiff equation integration problem in which the integration method must be able to follow fast transients by taking small integration steps. To complete the solution of the other transients, it must also rapidly increase its time step when initial transients have died out.

Unfortunately standard integration algorithms become numerically unstable when the step size is increased beyond that necessary to follow the fast transients. An alternative approach has been to replace the concentrations of fast reacting species by steady state approximations and integrate only the slow species. However, this method is at best approximate, and particularly in chemical equations can be grossly inaccurate due to the nonlinearities[1].

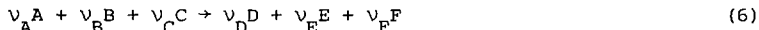
The backward differencing method proposed by Curtis and Hirschfelder[2] for stiff differential equations effectively avoided the stability constraint on integration step size, and an algorithm published by Gear[3] combining this with an effective error controlled step size and order selection has come into widespread use in a variety of scientific disciplines.

Extensions of this algorithm by Hindmarsh[4] recognize that the efficiency of computation is directly relatable to the accuracy and speed of evaluating and inverting the Jacobian matrix used in the predictor corrector equation, and provide various options for doing this. Carver and Baudouin[5] further improved efficiency for large equation systems by handling and storing the Jacobian as a sparse matrix, and optimizing its evaluation using the sparse routines of Curtis and Reid[6]. This sparse algorithm has been used with great success in the FORSIM simulation package[7,8] for some time, and has been further extended in MAKSIM to use the analytical expression of the Jacobian.

1.3 General Statement of Kinetics Equations

It is tedious to convert manually a large set of chemical reactions into the equivalent set of differential equations, and the process is prone to human error; however, the method may be readily defined in explicit mathematical terms and automated, thus eliminating error and maximizing efficiency.

Generalizing equations (1) to (4), a reaction, *i*, such as



where ν are integers, removes (-) reagents A, B and C from the system to form (+) products D, E and F at a rate

$$R_i = \pm k_i [A]^{\nu_A} [B]^{\nu_B} [C]^{\nu_C} = \pm k_i \prod_{j=1}^3 [x_j]^{\nu_j} \quad (7)$$

where k_i is the rate constant and square brackets denote concentration. Thus in m such reactions, each involving p_i species, the time derivative for the concentration of specie X_{g_i} is

$$\frac{d[X_{g_i}]}{dt} = \sum_{i=1}^m v_{x_{g_i}} R_i = \sum_{i=1}^m \pm k_i v_{x_{g_i}} \prod_{j=1}^{p_i} [X_{i_j}]^{v_{x_{i_j}}} \quad (8)$$

Furthermore, the elements of the associated Jacobian matrix also follow directly as

$$\frac{\partial}{\partial [X_r]} \frac{\partial [X_{g_i}]}{\partial t} = \sum_{i=1}^m k_i v_{x_{g_i}} v_{x_{r_i}} [X_{r_i}]^{(v_{x_{r_i}} - 1)} \prod_{\substack{j=1 \\ j \neq r}}^{p_i} [X_{i_j}]^{v_{x_{i_j}}} \quad (9)$$

Thus, not only can the differential equations be assembled from (8) but the exact analytic expression for the Jacobian (9) is available to use directly in the predictor-corrector equation.

1.4 Application Programs

The computer program WR20[9] obtained from the Argonne Code Centre, has been in use at CRNL for some time. It has a convenient user interface for reading the chemical equations and associated data, and automatically assembles the differential equations as in equations (6) to (8). It is, however, restricted to two reagents per reaction and is unable to integrate large equation sets efficiently.

When WR20 was tried on a set of 31 reactions involving only 11 species to model the radiolysis of water, it was unable to complete the calculation without using an exorbitant amount of computer time. The chemical equations were then converted manually to explicit differential equations and these were solved by the FORSIM package. A solution complete to 10^5 seconds problem time was completed in 2 seconds CDC 175 computer time in FORSIM, whereas WR20 required 5000 seconds to complete only 10 seconds of problem time on the same CDC 175 computer[10].

At this point, it was decided there was great potential in combining the WR20 input and equation assembly with the FORSIM sparse matrix integration algorithm, GEARZ, and a prototype program, CHEMIST, (CHEMical EQUation MANipulation and INTEGRation using STIFF Techniques) emerged as an uneasy marriage between the two. It performed the same calculation in approximately three times the time required by FORSIM. Part of this excess is inevitable because of the overhead involved in computing the differential equations in general form (8) rather than explicitly defining each equation as in FORSIM. The remainder was due to incompatibilities in the interface between GEARZ and WR20. A further difficulty arose in

determining the storage required, and fixing the maximum numbers of reagents, reactions and sampling times. These numbers varied widely between applications and no sensible maxima could be found which did not also make the program far too large for small applications. It was, therefore, decided to make the program entirely dynamic. It was completely rewritten in modular form, subject to the only restriction that the old WR20 data decks, a considerable accumulated collection, could be used with the new program. This new program, MAKSIMA-CHEMIST, which will henceforth be called MAKSIM, contains 34 subroutines, 17 of which relate directly to the chemistry and user interface, 12 to the integration process, and 5 to Calcomp and printer plotting.

Further details of the integration algorithm are given in references [8] and [11]. Comparisons with similar available packages, and validation tests to confirm the accuracy of the integrator and to illustrate its efficiency are described in [8] and comparisons with experimental data are discussed in [12].

2. DATA INPUT

The data input is designed to be compatible with WR20, that is to say, WR20 decks may be read into MACKSIM without major modification and vice-versa. Data are arranged into blocks, each of which perform a specific function. Blocks in MAKSIM are introduced by a *KEYWORD* card and ended by a blank card.

The keywords must be punched with the first * in column 1, and are as follows:

<u>Key</u>	<u>Data</u>
REACTIONS	chemical equation data block
SPECIES	species, initial conditions, etc. block
TIMING	dose rate function block
CHANGE	options and changes block
CCPLOT	Calcomp plot block
PRPLOT	printer plot block
TAPEOUT	tape output block
TAPEOUT2	special tape block
EXECUTE	commence execution
NEWDECK	commence complete new input deck
FINIT	terminate, no more data follows

The order of blocks is subject to the restrictions that the first three blocks are mandatory input. They may be read in any order but must precede the other blocks as the optional blocks may refer to them.

Each block contains a number of cards of which the last one must be blank.

Any number of textual comment cards may precede the data blocks, but cards within the blocks must contain the data in formats described below. The keyword blocks may contain other textual comment in columns 15-80.

2.1 The Mandatory Blocks

REACTIONS introduces the reaction equation cards. One card follows for each chemical reaction, and its associated rate constant. The format is compatible with WR20 for standard WR20 reactions which contain exactly two reagents, one to four products, and the rate constant. However, MACKSIM has considerably more flexibility, also permitting reactions with only one reagent, pseudo second order reactions, and third order reactions. The format is as follows:

<u>Column</u>	<u>Format</u>	<u>Symbol</u>	<u>Entry</u>	<u>Mandatory or Default Value</u>
1-5	A5	R1	First reacting species name	m
6	A1		+ sign	blank
7-11	A5	R2	Second reacting species name	blank
12	A1		= sign	=
13-17	A5	P ₁	First product species name	m
18	A1		+ or - sign associated with P ₂	blank
19-23	A5	P ₂	Second product species name	blank
24	A1		+ or - sign associated with P ₃	blank
25-29	A5	P ₃	Third product species name	blank
30	A1		+ or - sign associated with P ₄	blank
31-35	A5	P ₄	Fourth product species name	blank
36-45	E10.3	K	Reaction rate constant	m
46-49			blank	
50	A1		* sign	blank
51-55	A5	C	Catalyst or third reacting species name	blank

These cards may describe six types of reaction (see Section 3).

In order to monitor the production of any individual reaction, it is also possible to include a dummy product, D, in the reaction which is unique to that reaction. This species D should also be included in the species list, with zero initial value, and MACKSIM will then record the integrated production of the reaction as the concentration of D.

The final card must be blank.

SPECIES introduces the species block. One card follows for each species, giving its name, initial concentration, radiation yield and other associated data.

<u>Column</u>	<u>Format</u>	<u>Symbol</u>	<u>Entry</u>	<u>Mandatory or Default Value</u>
1-5	A5	S	Species name	m
6-10	I5	Ch	Species charge	0
11-20	E10.3	G	Radiation yield	0
21-30	E10.3	F	Rate of spontaneous formation, or input rate	0
31-40	E10.3	C_i	Initial concentration	0
41-50	E10.3	E_q	Equivalent conductance	0
51-60	E10.3	Ex	Molar absorptivity	0
64	I1	KON	Enter non zero to hold concentration at C_i throughout.	0

Any number of cards may be entered, the last card must be blank.

TIMING introduces the timing block. Cards following specify the variation of irradiation dose and/or the times at which interim printouts are required.

<u>Column</u>	<u>Format</u>	<u>Symbol</u>	<u>Entry</u>	<u>Mandatory or Default Value</u>
1-10	E10.3	TI	Next problem time	m
11-20	E10.3	DR	Mean dose rate from zero or previous TI to this TI.	0
71-75	I5	IREP	Repetition factor	1

1 < IREP < 1000 is permitted on 1 card only, say the mth card. The calculation and dose profile to that point is repeated IREP times, permitting a cyclical dose profile to be entered. Note TI(M+1) must exceed T(M)*IREP.

The remainder of the card is unused. Any number of timing cards may be entered but at least one is necessary. The final TI is the time at which calculation terminates and will henceforth be referred to as TFIN. The last card of the set must be blank.

2.2 Optional Blocks

CHANGE: This block may be used to change MAKSIM system options or previous data block items. On completing the mandatory blocks and again immediately after completing the post run options for each run, the program scans for change cards. If *CHANGE* is encountered, the following cards are used to introduce one change each.

<u>Column</u>	<u>Format</u>	<u>Symbol</u>	<u>Entry</u>
1-2	A2	PROP	Code as below
3-10	I8	INDEX	Index
11-20	E10.3	VALNEW	New value
41-80			Any textual comment

<u>Code</u>	<u>Change</u>	<u>Default</u>
RN	Run identification number = INDEX	1
KK	Rate constant of reaction (INDEX) = VALNEW	as read
GG	Radiation yield of species (INDEX) = VALNEW	as read
CI	Initial concentration of species (INDEX) = VALNEW	as read
EX	Initial concentration of species (INDEX) = VALNEW	as read
DR	Dose rate at all times = previous dose * VALNEW	as read
EP	Tolerable relative error	1.0E-5
TL	Minimum integration step	1.0E-25
YS	Value at which concentration is deemed to be effectively zero	1.0E-15
DS	Value below which a concentration derivative is deemed effectively insignificant	1.0E-10
DP	Maximum time between printouts	TFIN
NC	Number of output columns	10
MF	Integration option	MAKSIM selects
MA	Reaction matrix option IMA = INDEX	0
GV	Yield option IGV = INDEX	0
RE	If INDEX $\leq$ the current number of reactions (NR), an existing reaction is to be redefined. If INDEX > NR, a new reaction is to be defined, and NR is set = NR+1. In either case a single reaction is read in block 1 format. It should not contain new species however. In either case, a reaction card follows in reaction format.	

A blank card terminates the block. A change block is not mandatory for the first case run.

If results are to be recorded on tape for retention or further analysis, or plots are required, further data cards are necessary.

TAPEOUT: Tape recorder block: The key card is followed by up to five cards format 16A5 containing the names of species for which concentrations or yields are to be recorded on tape 8 using the format given in Section C. A blank card terminates the block.

CCPLOT - Calcomp plot block: The key card is followed by up to five cards, one for each plot frame. A blank card terminates the block.

Column	Format	Symbol	Entry
1-25	5A5	SCC	One to five species to be plotted.
26-30	I5	IYIELD	If > 0 , plot concentrations vs time. If < 0 , plot yields vs time.
31-60	3A10		Title of plot frame.
61-70	A10		x-axis units (time) default seconds.
71-80	A10		y-axis units (yields or concentrations) default mole/litre.

PRPLOT - Printer Plot Block: The key card is followed by data in the same form as the Calcomp plot block.

TAPEOUT2 is a special format tape output for existing undocumented plotting programs used by Physical Chemistry Branch.

EXECUTE This card is used to trigger execution of the run specified by all the data read in up to this point.

NEWDECK - This card indicates that a complete new data set will be read in, and deactivates all previous data.

FINIT - This indicates end of data and terminates smoothly.

Sample Input Deck

Actual input decks are given with the applications examples, Section 4. However, the structure is always similar:

Comment cards (if any)

```

:
:
*REACTIONS*
:
:
blank
*SPECIES*
:
:
blank
*TIMING*
:
:
blank
*CHANGE*
:
:

```

```
blank
*EXECUTE* (CASE 1)
*CHANGE*
:
:
blank
*TAPEOUT*
:
:
blank
*EXECUTE* (CASE 2)
*FINIT*
```

The above structure would run two cases. A *CHANGE* card is included even in the first case to change an optional parameter. After this execution, a further change is made and a tape will be made of results from the second case. Note that plot and tape blocks remain in effect once introduced, but may be deactivated by entering a keyword card followed immediately by a blank.

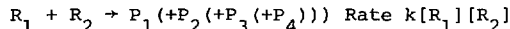
The finish could be replaced by *NEWDECK* followed by a new complete data set.

3. DISCUSSION OF INPUT DATA AND OPTIONS

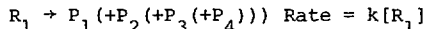
3.1 Chemical Reaction Specification

Although the input format appears rigid, it can in fact apply to seven distinct types of reaction. These are specified as follows:

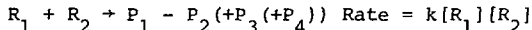
(a) Standard Second Order Reaction:



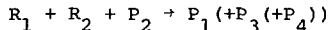
(b) First Order Reaction:



(c) Pseudo Second Order Reaction: Specified as

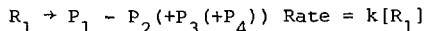


the reaction is actually

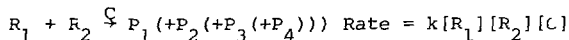


P_2 is consumed, but its concentration does not affect the rate.

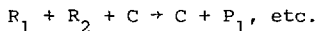
(d) Psuedo First Order Reaction:



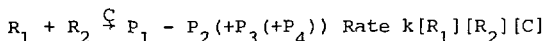
(e) Catalytic Second Order Reaction:



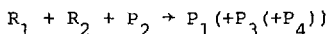
C affects the reaction in an ideal catalytic sense but is not consumed or created by it.



(f) Third Order Reaction:



when $C = P_2$ this is true third order reaction.



(g) Catalytic Third Order Reaction:

If $C \neq P_2$ in (f), this is a catalytic pseudo third order reaction. The first six types occur in the examples of section 3. This last has not been encountered in practice.

The rather awkward specification of the true third order reaction is necessitated by the restriction that input should be compatible with WR20. Actually, this is no great penalty as the great majority of reactions encountered will be second order.

3.2 Units

Units are not specified, as any self consistent set of units is satisfactory. A common choice is the following:

k	L.mol ⁻¹ .s ⁻¹ (second-order reaction)
G	molec. ⁻¹ .(100 eV) ⁻¹
F	mol.L ⁻¹ .s ⁻¹
C _i	mol.L ⁻¹
E _q	mho.mol ⁻¹ .L ⁻¹
Ex	L.mol ⁻¹ .cm ⁻¹
TI	s
DR	eV.L ⁻¹ .s ⁻¹

These units appear on all printout regardless of the actual unit set chosen, but units of variables appearing on plots may be specified on plot data cards.

3.3 Optional Parameters

RN - Run Index

If not entered, RN starts at 1 and increases 1 for each case.

EP - Relative Error Tolerance

In general it is advisable not to tamper with the integration algorithm. EP is roughly comparable to the number of accurate significant figures in the results, so 10^{-n} gives n reliable significant figures, thus EP should be between 10^{-3} and 10^{-10} , default is 10^{-5} .

TL - Minimum Time Step

There is little to be gained by increasing TL, as step size control is efficient. For exceptionally short-lived transients, TL may be decreased.

YS,DS - Significant Levels

These are the values at which concentration, and the concentration derivative, are deemed insignificant. The default values are adequate for problems in which expected concentrations do not greatly exceed 1.0. If the unit system is such that concentrations are very large or very small numbers, proportionately adjusting YS and DS will improve efficiency.

DP - Maximum Printout Limit

Printouts are normally given at the times indicated on the block 3 time cards. DP is used to apply a maximum time interval between prints if there are few time cards. Alternatively, if DP is entered negative, MAKSIM will print $|DP|$ times in linear intervals between each time card, or if DP = -1, approximately a page (60 lines) of output will be printed.

NC - Output Columns

Output is arranged in columns, one for each species, a row for each printout time. NC=10 is good for wide paper, 5 for narrow.

MF - Integration Method

A number of integration options are available within the GEARZ algorithm. If MF is left zero, MAKSIM will choose the option most appropriate for the available field length and the sparsity of the Jacobian matrix. The user may select one of the following values for MF:

- 1 No Jacobian analysis
- 2 Diagonal Jacobian approximation
- 3 Full numerical Jacobian approximation
- 4 Sparse numerical Jacobian approximation
- 5 Full analytical Jacobian approximation
- 6 Sparse analytical Jacobian approximation

If the user makes a choice requiring excess storage, MAKSIM will choose otherwise.

MA

The reaction matrix graphically illustrates the occurrence of species throughout the reaction set and may be used to check the chemical equations.

GV

Activates the option to print yields for each species, as well as concentrations.

TAPEOUT

If there are NT tape out cards with NS species requested, each card generates a data block of concentrations or yields LT entries long where LT is the number of printout times. Format is (NS+1)(E10.3).

From Card 1

T(1),C(T(1),NS₁₁),C(T(1),NS₁₂), ...
:
:
T(LT),C(...

From Card 2

T(1),C(T(T(1),NS₂₁),C(T(1),NS₂₂), ...
:
:
End File

From Card 1 next case

T(1),C...

The fact that .(1) is always zero allows the blocks associated with each card to be readily identified by subsequent processing programs.

4. APPLICATIONS

We now present three examples to illustrate the use of MAKSIM.

4.1 Cesium Flare Problem

This 10-reaction problem, originated by Edelson[15] has come to be regarded as a useful benchmark[13-16], as the species concentrations span 12 orders of magnitude during the evolution, and one component, O_2 , exhibits pseudo steady state behaviour for a short interval in the middle of the calculation. Table 1 gives the required information. Because this problem contains third order reactions, it was not possible to attempt the calculation using WR20, but MAKSIM uses the 'catalyst' concept.

Table 2 shows the required input data for a requested tolerance of 10^{-5} , MAKSIM exactly computes the five figure accurate results quoted as standard, and maintains a charge balance within 10^{-8} of the smallest concentration. The plot obtained is shown in Figure 1 and detailed results are given in the program output shown in Table 3. The computation takes less than a second on the CDC 170 Model 175 computer.

4.2 The Radiolysis of Water

The radiolytic decomposition of water is important to both moderator and coolant chemistry in nuclear reactors. The MAKSIM program has been used for extensive work in modelling the radiolysis of water, and the results have been successfully compared to the experimental data of Hochanadel[17], Schwarz[18] and others. Detailed comparisons are given by Boyd, Carver and Dixon[19]. Input to MAKSIM for the 39-equation, 11-species model is shown in Table 4. Three cases are requested, changing the initial pH value each case. A printer graph of several of the species is requested for each case and the first is shown in Figure 2. Computation time to follow this transient for 10^6 seconds is approximately 2 seconds.

4.3 Photochemical Smog Chamber

To test the package for a fairly large reaction set, we have used the 81 reaction model of a photochemical smog chamber discussed by Farrow and Edelson[1]. This 50-species model is also discussed by Stabler and Chesick[13]. Using the original Gear algorithm the latter must request a tolerance of 10^{-8} to obtain 10^{-5} relative error in concentration values, requiring 26.5 minutes to complete the calculation on an IBM 360/44 computer. MAKSIM maintains a 10^{-5} relative error for a 10^{-5} requested tolerance, requiring approximately 23 seconds on a CYBER 170/175. This time ratio of 68 considerably exceeds the expected speed ratio between the two machines, which is about 25.

The reaction set is extensive, and documented fully in [1], so it is reproduced here only as an input data deck in Table 5. Figure 3 shows the transient behaviour of four of the relevant species and may be compared to Figure 1 in [1]. Table 6 shows some comparative timing results. Note that use of the sparse matrix integration option reduces computing time by 50%. MAKSIM chooses this option for equation sets exceeding 25 species.

5. THE MAKSIM PROGRAM

The Overall Flowchart for MAKSIM is shown in Figure 4.

The program itself merely calls the executive subroutines, their function is as follows:

SIZER

SIZER predigests the input and determines whether all mandatory blocks are present. It then computes the required working storage and selects a suitable integration method.

PULLIN

PULLIN reads the mandatory data input blocks and assigns data to the storage areas allocated by SIZER.

SETUP

This routine performs initialization calculations and assures all optional parameters are set to appropriate values. It then sets up the array of reaction coefficients used to assemble equation 8, and prints the reaction coefficient matrix if requested.

PUTOUT

This reports on the initialized data set immediately prior to execution.

SOLVER

SOLVER directs the integration from start to finish by calling STIFFZ recording results as requested by calling routine STORE.

STIFFZ

The integration meta-algorithm is described in full in reference 8.

STIFFZ loads and calls a number of auxiliary routines, some of which may also be used independently. They are:

GEARZ	- Gear's algorithm	MF
COSET	- Coefficients for GEARS	all
DECOMP	- Decompose a full matrix	3
SOLVE	- Solve equations from DECOMP	3
JACOB	- Determine and pack a sparse Jacobian	4
SPARSE	- Decompose a sparse matrix	4-6
SPARSEB	- Solve equations from SPARSE	4-6
SORTAG	- Sort an array of numbers	4-6

For MAKSIM, STIFFZ also calls the following three routine pairs:

DIFFUN/DIFFON - assemble differential equations (8)
JACOBI/JACOBJ - assemble analytical Jacobian matrix from equation (9)
JACOBS/JACOBT - assemble analytical Jacobian matrix from equations (9) treating the matrix as sparse.

STORE

This routine stores results for post run processing.

RESULT

RESULT processes the stored results on completion of an integration run. It calls the plot routines if necessary.

ALTER

This routine changes the options as requested by the *CHANGE* key card.

READSP

READSP reads data for the CCLOT, PRLOT and TAPEOUT blocks.

CCLOT

CCLOT is the Calcomp plot executive routine. It calls CRNL library software to produce the Calcomp plots.

PRLOT

PRLOT produces the printer plots.

CONC and SCAN

CONC and SCAN manipulate characters.

PRGRID

PRGRID prints the Calcomp plot.

RECORD

RECORD records data for the *TAPEOUT* options.

QUITS

QUITS is the termination routine.

CHNGSCM and MYFL

CHNGSCM and MYFL interact with the CRNL system to implement dynamic storage.

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Table 1: Cesium Flare Reaction

Reaction		Rate Constant	Units
1.	$O_2^- \rightarrow O_2 + e^-$	4.00×10^{-1}	s^{-1}
2.	$Cs^+ + e^- \rightarrow Cs$	1.00×10^{-12}	$cm^3 \text{ molecule}^{-1} s^{-1}$
3.	$O_2 + e^- \rightarrow O_2^-$	1.40×10^{-16}	$cm^3 \text{ molecule}^{-1} s^{-1}$
4.	$O_2^- + Cs^+ \rightarrow Cs + O_2$	5.00×10^{-8}	$cm^3 \text{ molecule}^{-1} s^{-1}$
5.	$Cs \rightarrow Cs^+ + e^-$	3.24×10^{-3}	s^{-1}
6.	$O_2 + 2Cs \rightarrow CsO_2 + Cs$	1.00×10^{-31}	$cm^6 \text{ molecule}^{-2} s^{-1}$
7.	$O_2 + Cs + CsO_2 \rightarrow 2CsO_2$	1.00×10^{-31}	$cm^6 \text{ molecule}^{-2} s^{-1}$
8.	$O_2 + Cs \rightarrow CsO_2$	1.40×10^{-16}	$cm^3 \text{ molecule}^{-1} s^{-1}$
9.	$2O_2 + Cs \rightarrow CsO_2 + O_2$	1.00×10^{-31}	$cm^6 \text{ molecule}^{-2} s^{-1}$
10.	$2O_2 + e^- \rightarrow O_2^- + O_2$	1.24×10^{-30}	$cm^6 \text{ molecule}^{-2} s^{-1}$

Species	Concentrations - Molecule cm^{-3}	
	t=0	t=1000
1. e^-	1.0×10^2	4.9633×10^4
2. O_2^-	5.2×10^2	2.5904×10^4
3. Cs^+	6.2×10^2	7.5622×10^4
4. Cs	1.0×10^{12}	1.5319×10^3
5. CsO_2	0.0	1.000×10^{12}
6. O_2	3.6×10^{14}	3.5900×10^{14}

TABLE 2

INPUT DECK FOR EXAMPLE 1

CARD COLUMNS		1	6	1	6	1	6	1	6	1	6	1	6
MAKSIM EXAMPLE 1		1	6	1	6	1	6	1	6	1	6	1	6
REACTIONS													
O2-	=O2	+E-			4.000E-01								
CS+	+E-	=CS			1.000E-12								
O2-	+E-	=O2-			1.400E-16								
O2-	+CS+	=CS	+O2		5.000E-08								
CS	=CS+	+E-			3.240E-03								
O2	+CS	=CSO2			1.000E-31			CS					
O2	+CS	=CSO2			1.000E-31			CSO2					
O2	+CS	=CSO2			1.400E-16								
O2	+CS	=CSO2			1.000E-31			O2					
O2	+E-	=O2-			1.240E-30			O2					
SPECIES													
E-	-1				1.000E+02								
O2-	-1				5.200E+02								
CS+	+1				6.200E+02								
CS					1.000E+12								
CSO2													
O2					3.600E+14								
TIMING													
					1.000E-03								
					1.000E+00								
					1.000E+03								
CCPLOT													
O2-	CS+	CS	CSO2		FIG.1	CESIUM FLARE MODEL		SECONDS		MOLEC/CC			
CHANGE													
DP			-10.										
EXECUTE													
FINIT													

Table 3: Output from Cesium Flare Problem

```

*****
MACKSINA-CHEMIST
MASS ACTION CHEMICAL KINETICS SIMULATION - AUTOMATIC
CHEMICAL EQUATION MANIPULATION AND INTEGRATION USING
SPARSE TECHNIQUES
AUTHORS MIKE CARVER AND DON HANLEY
MATHEMATICS AND COMPUTATION BRANCH
CHALK RIVER NUCLEAR LABORATORIES
SUMMER OF 78
*****

```

INPUT DATA BLOCKS AND TEXTUAL COMMENTS ENCOUNTERED

```

TABLE 2      INPUT DECK FOR EXAMPLE 1
CARD COLUMNS
1 6 1 6 1 6 1 6 1 6 1 6
MAXIMUM EXAMPLE 1 CESIUM FLARE MODEL
*REACTIONS*
*SPECIES*
*INITIAL*
*CC*
*CHANGE*

```

OPTION CHANGES FOR THIS CASE
 DP = 8 IS CHANGED TO -1.000E+01
 EXECUTE = 0

BLANK COMMON SIZE REQUIRED 1239 FIELD LENGTH 24229(0000057245B) JOB CARD FIELD LENGTH IS 32768(0000000000B)
 *** WILL USE METHOD 5 FULL ANALYTIC MATRIX ANALYSIS TO INTEGRATE 6 EQUATIONS

79-01-16

NO	REACTION	RATE CONSTANT	CATALYST
1	O2- = O2 + E-	K(1) = 4.000E-01	*
2	CS+ + E- = CS	K(2) = 1.000E-12	*
3	O2 + E- = O2-	K(3) = 1.400E-16	*
4	O2- + CS+ = CS + O2	K(4) = 5.900E-08	*
5	CS + E- = CSO2	K(5) = 3.240E-03	*
6	O2 + CS = CSO2	K(6) = 1.000E-31	*CS
7	O2 + CS = CSO2	K(7) = 1.000E-31	*CSO2
8	O2 + CSO2 = O2 + CS	K(8) = 1.400E-16	*
9	O2 + CS = CSO2	K(9) = 1.000E-31	*O2
10	O2 + E- = O2-	K(10) = 1.240E-30	*O2

NO	SPECIES	CHARGE	G	S	CI	EQCO	EXT	SKIP
1	E-	-1	0.000	0.	0.	0.	0.	0
2	O2-	-1	0.000	0.	5.200E+02	0.	0.	0
3	CS+	1	0.000	0.	6.200E+02	0.	0.	0
4	CS	0	0.000	0.	1.000E+12	0.	0.	0
5	CSO2	0	0.000	0.	0.	0.	0.	0
6	O2	0	0.000	0.	3.600E+14	0.	0.	0

NO	TIME	DOSE RATE
1	1.000E+03	0.
2	1.000E+00	0.
3	1.000E+03	0.

CONCENTRATIONS OF SPECIES:

TIME	E-	O2-	CS+	CS	CSO2	O2	COND	ABSC	DT	CHSUM
SECONDS	MOL/L	MOL/L	MOL/L	MOL/L	MOL/L	MOL/L	HKG/CM	/CM	S	UNITS
0.	0.	5.200E+02	6.200E+02	1.000E+12	0.	3.600E+14	0.	0.	1.000E-25	1.000E+02
1.000E-04	3.240E+05	5.234E+02	3.240E+05	1.000E-12	6.340E+06	3.600E+14	0.	0.	1.000E-04	1.000E+02
2.000E-04	6.480E+05	5.336E+02	6.480E+05	1.000E-12	1.260E+07	3.600E+14	0.	0.	1.000E-04	1.000E+02
3.0E-04	9.720E+05	5.587E+02	9.720E+05	1.000E-12	1.982E+07	3.600E+14	0.	0.	1.000E-04	1.000E+02
4.000E-04	1.296E+06	5.746E+02	1.296E+06	1.000E-12	2.536E+07	3.600E+14	0.	0.	3.277E-04	1.000E+02
5.000E-04	1.620E+06	6.054E+02	1.620E+06	1.000E-12	3.170E+07	3.600E+14	0.	0.	3.277E-04	1.000E+02
6.000E-04	1.944E+06	6.430E+02	1.944E+06	1.000E-12	3.804E+07	3.600E+14	0.	0.	3.277E-04	1.000E+02
7.000E-04	2.268E+06	6.876E+02	2.268E+06	1.000E-12	4.430E+07	3.600E+14	0.	0.	3.277E-04	1.000E+02
8.000E-04	2.592E+06	7.385E+02	2.592E+06	9.999E+11	5.072E+07	3.600E+14	0.	0.	3.277E-04	1.000E+02
9.000E-04	2.916E+06	7.967E+02	2.916E+06	9.999E+11	5.705E+07	3.600E+14	0.	0.	3.277E-04	1.000E+02
1.000E-03	3.240E+06	8.616E+02	3.240E+06	9.999E+11	6.339E+07	3.600E+14	0.	0.	3.277E-04	1.000E+02
1.000E-01	3.224E+08	2.325E+06	3.247E+08	9.933E+11	6.375E+09	3.600E+14	0.	0.	7.824E-03	1.000E+02
2.000E-01	6.329E+08	3.976E+06	6.368E+08	9.067E+11	1.264E+10	3.600E+14	0.	0.	9.597E-03	1.000E+02
3.000E-01	9.347E+08	4.160E+06	9.389E+08	9.002E+11	1.807E+10	3.600E+14	0.	0.	1.436E-02	1.000E+02
4.000E-01	1.228E+09	4.175E+06	1.332E+09	9.737E+11	2.505E+10	3.60E+14	0.	0.	1.703E-02	1.000E+02
5.000E-01	1.519E+09	4.187E+06	1.513E+09	9.673E+11	3.121E+10	3.60E+14	0.	0.	2.231E-02	1.000E+02
6.000E-01	1.792E+09	4.192E+06	1.795E+09	9.609E+11	3.731E+10	3.600E+14	0.	0.	2.231E-02	1.000E+02
7.000E-01	2.060E+09	4.196E+06	2.064E+09	9.546E+11	4.330E+10	3.600E+14	0.	0.	4.746E-02	1.000E+02
8.000E-01	2.321E+09	4.199E+06	2.325E+09	9.483E+11	4.940E+10	3.600E+14	0.	0.	4.746E-02	1.000E+02
9.000E-01	2.575E+09	4.201E+06	2.578E+09	9.420E+11	5.538E+10	3.599E+14	0.	0.	9.361E-02	1.000E+02
1.000E+00	2.821E+09	4.203E+06	2.826E+09	9.350E+11	6.132E+10	3.599E+14	0.	0.	9.361E-02	1.000E+02
1.000E+02	4.790E+07	3.405E+06	5.131E+07	1.085E+09	9.901E+11	3.590E+14	0.	0.	6.403E-01	1.000E+02
2.000E+02	1.271E+06	5.628E+05	1.034E+06	4.664E+06	1.000E+12	3.590E+14	0.	0.	2.647E+00	1.000E+02
3.000E+02	3.417E+05	1.710E+05	5.136E+05	9.742E+04	1.000E+12	3.590E+14	0.	0.	2.204E+00	1.000E+02
4.000E+02	1.874E+05	9.688E+04	2.816E+05	2.400E+04	1.000E+12	3.590E+14	0.	0.	2.204E+00	1.000E+02
5.000E+02	1.295E+05	6.637E+04	1.950E+05	1.002E+04	1.000E+12	3.590E+14	0.	0.	1.547E+00	1.000E+02
6.000E+02	9.761E+04	5.063E+04	1.403E+05	6.111E+03	1.000E+12	3.590E+14	0.	0.	1.033E+00	1.000E+02
7.000E+02	7.065E+04	4.000E+04	1.196E+05	3.818E+03	1.000E+12	3.590E+14	0.	0.	8.844E+00	1.000E+02
8.000E+02	6.503E+04	3.420E+04	1.002E+05	2.723E+03	1.000E+12	3.590E+14	0.	0.	1.542E+01	1.000E+02
9.000E+02	5.600E+04	2.951E+04	8.620E+04	2.091E+03	1.000E+12	3.590E+14	0.	0.	2.093E+01	1.000E+02
1.000E+03	4.963E+04	2.590E+04	7.562E+04	1.512E+03	1.000E+12	3.590E+14	0.	0.	2.757E+01	1.000E+02

TABLE 4

MAKSIM EXAMPLE 2
RADIOLYSIS OF WATER MODEL
INPUT DECK FOR 3 CASES OF DIFFERING INITIAL PH VALUES

REACTIONS		RATE CONSTANTS	
REACTIONS			
E- +O2	=O2-	2.000E+11	
E- +H2O2	=OH- +OH-	1.200E+11	
H +O2	=H2O	2.000E+11	
OH +H2	=H2O	3.300E+08	
OH +H2O2	=H2O +H2O	9.000E+08	
HO2 +HO2	=H2O2 +O2	6.000E+07	
O2- +O2-	=H2O2 +O2	5.100E+08	
OH +HO2	=H2O +O2	1.400E+11	
OH +OH	=H2O2	5.500E+10	
H +H2O2	=OH +H2O	2.700E+09	
E- +H+	=H	2.200E+11	
E- +HO2	=HO2-	2.000E+11	
H +HO2	=H2O2	2.000E+11	
E- +E-	=H2	5.000E+10	
E- +OH	=OH-	3.000E+11	
H +H	=H2	1.000E+11	
H +OH	=H2O	2.000E+11	
E- +H	=H2	2.500E+11	
OH +O2-	=O2 +OH-	8.000E+10	
H +OH-	=E- +H2O	2.100E+08	
E- +HO2-	=OH +OH-	3.500E+10	
H+ +OH-	=H2O	1.430E+12	
H+ +O2-	=HO2	5.000E+11	
HO2 +O2-	=O2 +HO2-	2.100E+09	
H +O2-	=HO2-	2.000E+11	
E- +O2-	=HO2- +OH-	3.000E+11	
OH- +H2O2	=HO2- +H2O	3.000E+09	
E- +H2O	=H +OH-	2.000E+02	
HO2- +H2O	=H2O2 +OH-	1.000E+05	
HO2	=H+ +O2	8.000E+06	
H2O2	=H+ +HO2-	3.560E-01	
H2O	=H+ +OH-	2.650E-04	
H+ +HO2-	=H2O2	2.000E+11	

SPECIE, CHARGE, YIELD INITIAL CONCENTRATION

SPECIES			
E-	-1	1.815E+00	
H		5.250E-01	
H2		6.650E-01	1.000E-05
OH-	-1	5.000E-02	1.000E-07
H+	+1	1.865E+00	1.000E-07
OH		1.920E+00	
HO2-	-1		
HO2		2.000E-02	
H2O2		8.450E-01	
O2-	-1		
H2O			5.554E+01

1

TIME	DOSE RATE
TIMING	
1.000E-05	1.180E+19
1.000E-03	1.180E+19
1.000E-01	1.180E+19
1.000E+01	1.180E+19
1.000E+03	1.180E+19

PRPLOT					
E- OH HO2 H2O2 H					
CHANGE				FIG.2	RADIOLYSIS OF WATER
				SECONDS	MOLE/LITRE
EXECUTE					
CHANGE				CASE 1	
CI 4	1.000E-06			CHANGES FOR CASE 2	
CI 5	1.000E-08				
EXECUTE				CASE 2	
CHANGE				CHANGES FOR CASE 3	
CI 4	1.000E-08				
CI 5	1.000E-06				
EXECUTE				CASE 3	
FINIT					

[illegible]

Table 6: Performance of Sparse Matrix Integrator
on Photochemical Smog Model

Jacobian Option Matrix Type Evaluation	Computing Times to 200 s Problem Time (seconds CDC Cyber 175)			
	Full Numeric	Full Analytic	Sparse Numeric	Sparse Analytic
Relative Error (Requested and Obtained)				
10^{-4}	45	42	33	19
10^{-5}	55	50	41	23
10^{-6}	67	54	51	30

FIG.1 CESIUM FLARE MODEL

□ OZ- △ CS+ x CS , CSO2

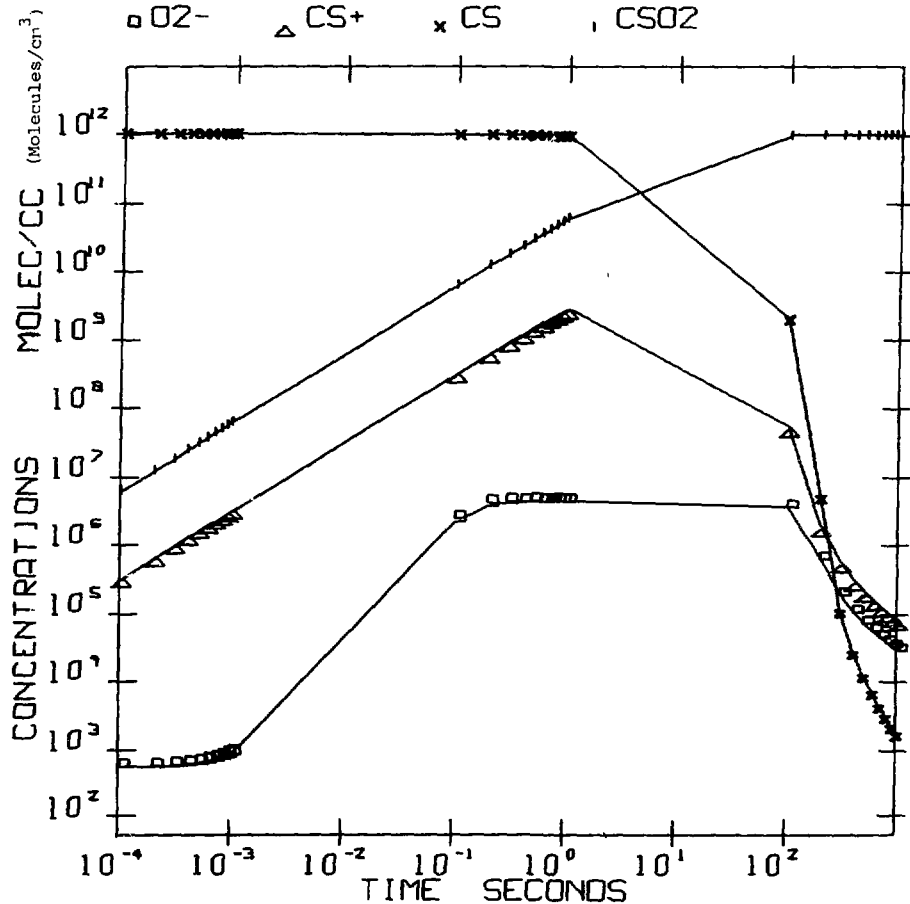


FIG.2 RADIOLYSIS OF WATER

SYMBOLS

* = E-
+ = OH
= HO2
- = H2O2
= H

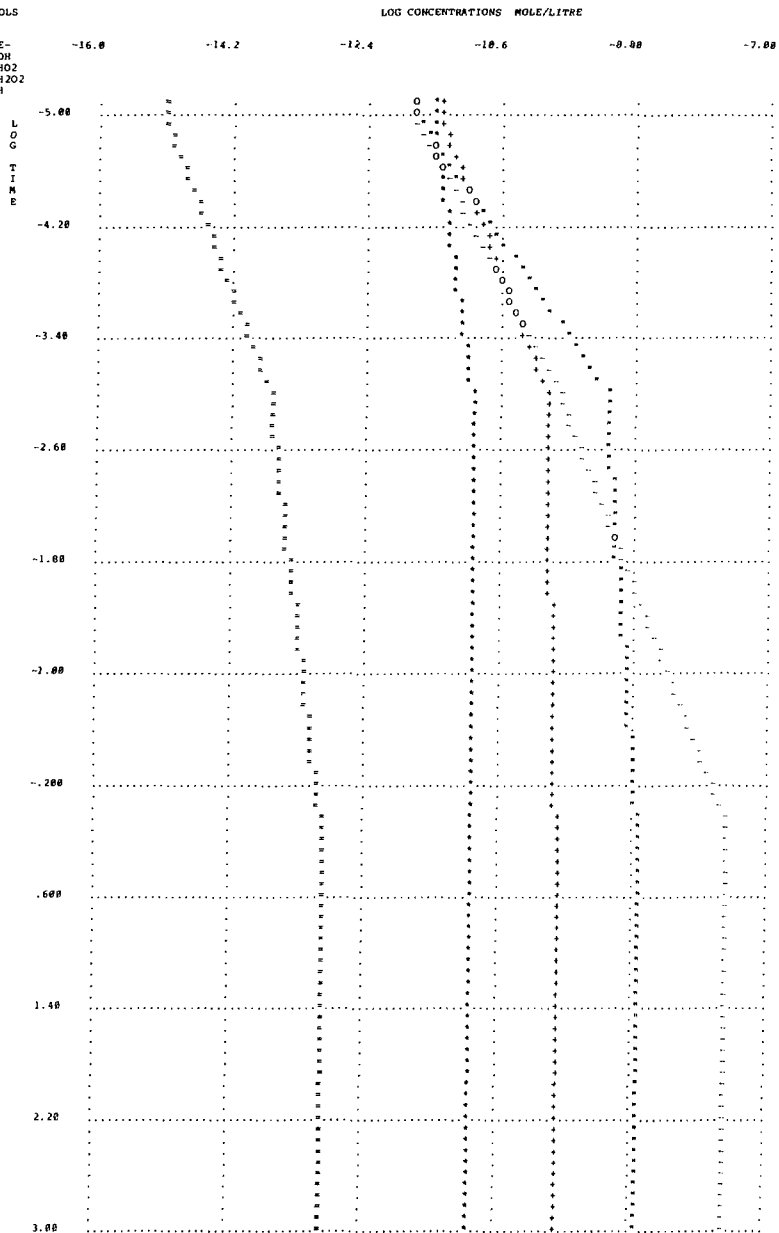


FIG.3 PHOTOCHEMICAL SMOG MODEL

□ NO₂ △ O₃ × C₃H₆ , NO

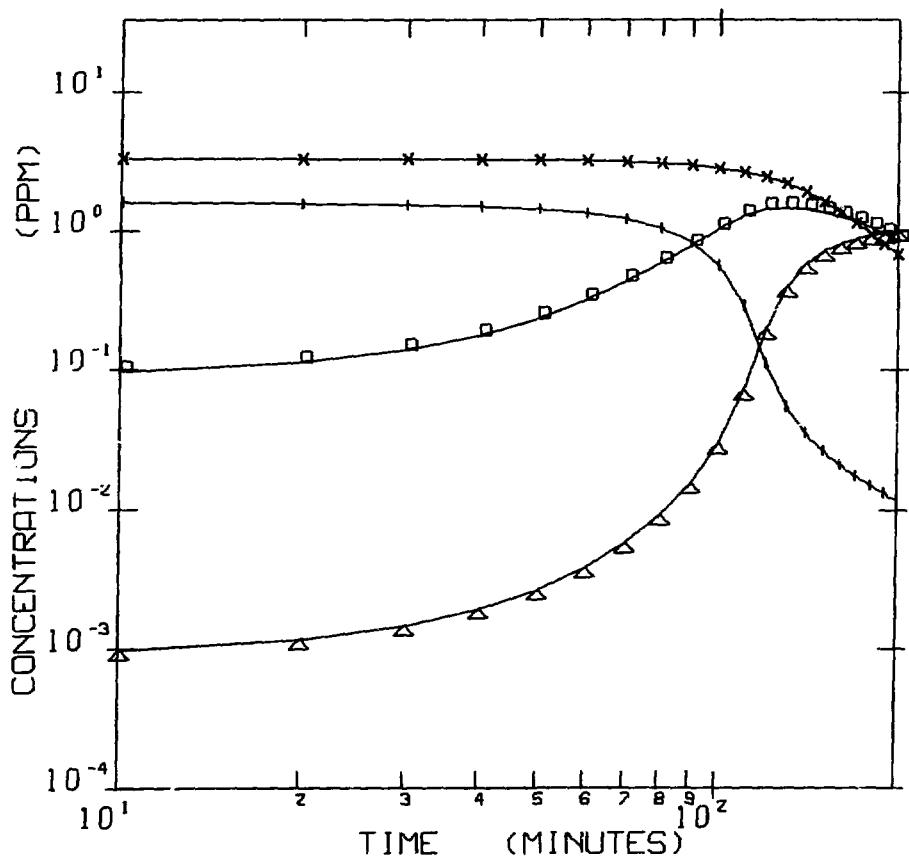
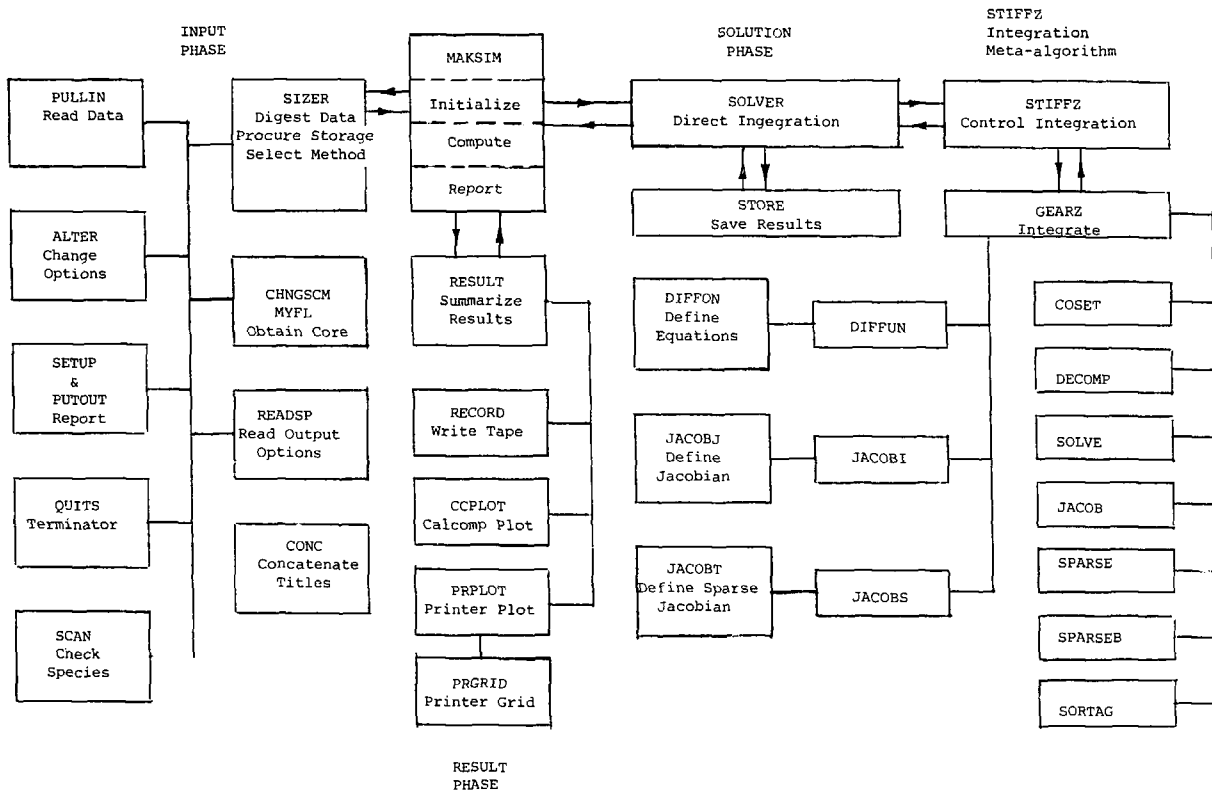


Figure 4: MAKSIM Organizational Chart



APPENDIX A
USE OF MAKSIMA-CHEMIST ON THE CRNL SYSTEM

The program is kept on permanent file in absolute form. Requisite control cards are:

JOB,...	User's job card
ATTACH,MAKSIM.	Access MAKSIM
MAKSIM.	Execute MAKSIM
7/8/9	End of record
Data	Data deck blocks
7/8/9	End of record
6/7/8/9	End of file

The program card is

```
PROGRAM MAKSIM(INPUT,OUTPUT,TAPE8,PLOT,TAPE5=INPUT,TAPE6=OUTPUT)
```

Tape 8 is reserved for recorded results and must be rewound if used for subsequent input. Input may be read from tape 5 or cards.

The sequence

```
MAKSIM(DISC1,,DISC2)  
REWIND(DISC2)  
DIGEST(DISC2)
```

reads input from file DISC1 and then uses the result file DISC1 as input to a subsequent program residing on local file DIGEST.



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