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RESULTS OBTAINED FROM THE FRICKE DIFFUSION KINETICS CODE

by

Erwin H. Bareiss, Cynthia Chamot,
and Hugo Fricke

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ABSTRACT

The Diffusion Kinetics codes described by the authors in ANL-6556 were used to study hypothetical reactions of free radicals produced by passing α rays and γ rays through aqueous solutions. Tables and graphs of results are given for about 200 cases run on the IBM 704 with various parameter combinations. Intermediate as well as final concentrations are given for some γ-ray cases.

INTRODUCTION

The IBM 704 Diffusion Kinetics codes[1] were used for over 200 cases to study from two to four primary reactions involving free radicals, and also a secondary reaction. Cases were run to determine values of various parameters, giving results, R_1 and R_2, consistent with those obtained experimentally for water and for water:iodine:iodide systems. Other parameters were varied to study their effects. In this report, results are tabulated and a large number of graphs are included to illustrate various effects. Also, some results of the previous Avidac codes[2] are included for comparison.

Complete output was normally obtained; so reactions of interest may be traced over all space up to the time they were removed from the machine. Although most α-ray cases ($\epsilon = 1$ for cylindrical symmetry) were run until the reaction was complete, some of the first cases were not allowed to finish, but those reactions can be followed part way to $T = 0.001$. Complete output is available for several γ-ray cases ($\epsilon = 2$ for spherical symmetry) which were run to completion. However, it was profitable to stop many of these cases at $T = 0.1$, since final concentrations of reaction products could be obtained by extrapolation.

The actual reactions being considered were: $H + H = H_2$; $H + OH = H_2O$; and $OH + OH = H_2O_2$ in all three codes; and $H + I = H^+ + I^-$ and $OH + I^- = OH^- + I$ in code B only; and a secondary reaction, $OH + H_2O_2 = H_2O + HO_2$ in code C only.

For the machine codes, H = X_1, OH = X_2, I = X_3, I^- = X_4, and H_2O_2 = X_4*. The amounts of reaction products formed are F_{11} for H_2, F_{12} for H_2O, F_{22} for H_2O_2, F_{13} for H^+, F_{24} for OH^-, and F_{24}^* for HO_2.

The physical interpretations of the symbols are given in Table I. It should be noted that these are all dimensionless parameters. For further information, see Ref. 1.

Table I

SYMBOLS AND THEIR PHYSICAL MEANINGS

Input Parameters	
Symbol	Definition
β	A measure of the initial scatter of X_1 relative to X_2.
$\theta_i = D_i/D_1$	The diffusion rate for X_i relative to that of X_1.
$E = E_R$	A measure of the initial concentration of X_1. It should be noted that E_M referred to in references 2 and 3 would be $2E_R$.
ϵ	This is 1 for cylindrical symmetry (α rays) and 2 for spherical symmetry (γ rays).
γ_i	Ratio of the initial concentrations of the solutes to the concentration of X_1 at the origin.
$\kappa_{ij} = k_{ij}/k_{11}$	The rate of reaction for X_i combining with X_j relative to that of X_1 with X_1.
Problem Parameters	
Symbol	Definition
B_i	A measure of the initial concentrations of the solutes, X_3 and X_4, incorporated into γ_i for input data.
F_{ij}	Transformed fractional amounts of reaction products formed (or of free radicals remaining if j=0).
R	Position in transformed space, going from 1 at the center of the initial free radical concentrations, to 0 far away.
T	Transformed time, going from 1 at time of initial free radical formation, to 0 as real time t increases to ∞.
$U_i(R,T)$	Transformed concentrations of reactants X_i at various points in space at time T.
Experimentally Determined Quantities (at T = 0)	
Symbol	Definition
R_1	$F_{22}/F_{11} = 1.62$ for γ rays with no solute present.
R_2	$(F_{10} + F_{20})/(F_{11} + F_{22}) = 2.40$ for γ rays with no solute present.

Note: The subscripts i and j refer to the reactants X_1, X_2, X_3, or X_4. The ij combinations are limited to 11, 12, 13, 22, and 24.

SECTION ONE: FINAL RESULTS FOR α-RAY CASES (CYLINDRICAL GEOMETRY)

Table II gives certain standard parameter values which were common to several cases.

Table III gives some parameter combinations for which the computations were not completed, so that only intermediate results are available.

Table IV gives results for some cases based on Standard I.

Table V gives parameter combinations for cases based on Standard II, with six different values of E. It should be noted that for the smaller values of E, smaller values of B must be used to facilitate the normalizations of curves to B = 0.

Tables VI to XI give the final results for the cases in Table V.

Figures 1-22 are graphs of final F_{ij} vs. B and normalized F_{ii} vs. B_{i+2} for each value of E in Table V.

Table II

VALUES OF PARAMETERS FOR STANDARD α-RAY CASES

B_3 and B_4 vary.	ϵ	β	D_2/D_1	D_4/D_1 D_3/D_1	k_{12}/k_{11}	k_{24}/k_{11} k_{13}/k_{11}	k_{22}/k_{11}
STANDARD I	1	1	0.4545	0.15	2	2*	1
STANDARD II	1	1	0.25	0.15	2	2*	0.55

*It should be noted that for 2-radical cases only, k_{13}/k_{11} and k_{24}/k_{11} are set equal to zero.

Table III

PARAMETERS FOR PRELIMINARY α-RAY (ϵ = 1) CASES WITH TWO RADICALS ONLY (CODE A)

Case No.	β	E	D_2/D_1	k_{12}/k_{11}	k_{22}/k_{11}	
1-1	1	1.8	0.333	2	1	
1-2	1	1.8	0.50	2	1	
1-3	1	1.8	0.667	2	1	
1-4	1	1.8	1.0	2	1	
1-5	1	2.5	0.333	2	1	
1-6	1	2.5	0.50	2	1	
1-7	1	2.5	0.667	2	1	
1-8	1	2.5	1.0	2	1	
26	1	1.97	0.4545	2	1	Standard I

These cases were not computed all the way. Cases No. 1-1 to 1-8 were stopped at T = 0.001, when F_{10} and F_{20} were still near 0.05, and No. 26 was run until T = 10^{-16}, at which time F_{10} still exceeded 0.01.

Table IV

PARAMETERS AND FINAL RESULTS OF SOME FOUR-COMPONENT CASES BASED ON STANDARD I WITH E = 1.97 AND ϵ = 1 (FOR α RAYS)

Case No.	B_3	B_4	F_{11}	F_{12}	F_{13}	F_{22}	F_{24}
126	10^{-5}	10^{-5}	0.4565	0.4711	0.0724	0.5070	0.0219
127	10^{-3}	10^{-5}	0.4332	0.4567	0.1101	0.5034	0.0399
128	10^{-1}	10^{-5}	0.3312	0.3759	0.2929	0.4653	0.1588
129	1	10^{-5}	0.1788	0.2372	0.5840	0.4086	0.3542
130	10	10^{-5}	0.0404	0.0697	0.8899	0.3621	0.5682
126	10^{-5}	10^{-5}	0.4565	0.4711	0.0724	0.5070	0.0219
132	10^{-5}	10^{-3}	0.4540	0.4566	0.0894	0.4896	0.0538
133	10^{-5}	10^{-1}	0.4240	0.3778	0.1962	0.3778	0.2443
134	10^{-5}	1	0.3789	0.2387	0.3824	0.1951	0.5662
135	10^{-5}	10	0.3426	0.0699	0.5875	0.0413	0.8888

Table V

CASE NUMBERS OF α-RAY CASES WITH STANDARD II PARAMETERS AND SIX VALUES OF E FOR WHICH B_3 AND B_4 VARY

E = 5.305

B_3 \ B_4	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}
10	580				525		
1		581			526		
0.1			582		527		
10^{-3}				583	528		
10^{-5}	520	521	522	523	524		
10^{-7}							
10^{-10}							

E = 0.675

B_3 \ B_4	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}	10^{-15}
10	585				555			
1		586			556			
0.1			587		557			
10^{-3}				588	558			
10^{-5}	550	551	552	553	554		516	
10^{-10}					517		515	
10^{-15}								515A

E = 2.48

B_3 \ B_4	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}
10	505				535		
1		506			536		
0.1			507		537		
10^{-3}				508	538		
10^{-5}	530	531	532	533	534		
10^{-7}						509	
10^{-10}							

E = 0.3535

B_3 \ B_4	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}	10^{-15}
10	500				565			
1		501			566			
0.1			502		567			
10^{-3}				503	568			
10^{-5}	560	561	562	563	564		518	
10^{-10}					519		514	
10^{-15}								529

E = 1.29

B_3 \ B_4	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}
10							
1							
0.1							
10^{-3}							
10^{-5}	540	541	542	543	544	539	539A
10^{-7}							
10^{-10}							

E = 0.1875

B_3 \ B_4	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}	10^{-15}
10	590				575			
1		591			576			
0.1			592		577			
10^{-3}				593	578			
10^{-5}	570	571	572	573	574	595	579	597
10^{-10}					599			512
10^{-15}								

Table VI

RESULTS FOR STANDARD II AND E_R = 5.305 (E_M = 10.61)

Case No.	520	521	522	523	524
$B_3 = 10^{-5}$ B_4 =	10	1	0.1	10^{-3}	10^{-5}
F_{11}	0.35475	0.38508	0.40787	0.41951	0.42131
F_{12}	0.14213	0.36699	0.48859	0.53667	0.54404
F_{13}	0.5031	0.2479	0.1035	0.0438	0.0347
F_{22}	0.05295	0.21260	0.36252	0.43966	0.45048
F_{24}	0.8049	0.4204	0.1489	0.0237	0.0055

Case No.	525	526	527	528	524
$B_4 = 10^{-5}$ B_3 =	10	1	10^{-1}	10^{-3}	10^{-5}
F_{11}	0.08592	0.26192	0.37117	0.41371	0.42131
F_{12}	0.14327	0.36144	0.48488	0.53603	0.54404
F_{13}	0.7708	0.3766	0.1440	0.0503	0.0347
F_{22}	0.28252	0.35229	0.41697	0.44714	0.45048
F_{24}	0.5742	0.2863	0.0982	0.0168	0.0055

Case No.	580	581	582	583	524
$B_3 = B_4$ =	10	1	10^{-1}	10^{-3}	10^{-5}
F_{11}	0.08785	0.26150	0.36887	0.41355	0.42131
F_{12}	0.09246	0.30574	0.46292	0.53402	0.54404
F_{13}	0.8197	0.4328	0.1682	0.0524	0.0347
F_{22}	0.05369	0.20501	0.35512	0.43907	0.45048
F_{24}	0.8539	0.4893	0.1820	0.0269	0.0055

Table VII

RESULTS FOR STANDARD II AND E_R = 2.48 (E_M = 4.96)

Case No.	530	531	532	533	534
$B_3 = 10^{-5}$ B_4 =	10	1	0.1	10^{-3}	10^{-5}
F_{11}	0.34104	0.36493	0.39316	0.41169	0.41284
F_{12}	0.08548	0.28650	0.44167	0.51852	0.53033
F_{13}	0.5735	0.3486	0.1652	0.0698	0.0568
F_{22}	0.02886	0.14926	0.31906	0.43293	0.44942
F_{24}	0.8857	0.5642	0.2393	0.0486	0.0203

Case No.	535	536	537	538	534
$B_4 = 10^{-5}$ B_3 =	10	1	0.1	10^{-3}	10^{-5}
F_{11}	0.04871	0.19602	0.32785	0.39924	0.41284
F_{12}	0.08620	0.28473	0.43688	0.51771	0.53033
F_{13}	0.8651	0.5193	0.2353	0.0831	0.0568
F_{22}	0.27090	0.33118	0.40221	0.44568	0.44942
F_{24}	0.6429	0.3841	0.1609	0.0366	0.0203

Case No.	505	506	507	508	534	509
$B_3 = B_4$ =	10	1	0.1	10^{-3}	10^{-5}	10^{-7}
F_{11}	0.04862	0.19410	0.32542	0.39883	0.41284	0.41849
F_{12}	0.05036	0.22234	0.40597	0.51379	0.53033	0.53569
F_{13}	0.9010	0.5836	0.2686	0.0874	0.0568	0.0458
F_{22}	0.02874	0.14500	0.31140	0.43202	0.44942	0.45400
F_{24}	0.9209	0.6327	0.2826	0.0542	0.0203	0.0103

Table VIII

RESULTS FOR STANDARD II AND E_R = 1.29 (E_M = 2.58)

Case No.	540	541	542	543	544	539	539A
$B_3 = 10^{-5}$ B_4 =	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}
F_{11}	0.32624	0.34420	0.37382	0.39781	0.39950	0.39971	0.39971
F_{12}	0.05056	0.21258	0.38402	0.49168	0.51141	0.51345	0.51347
F_{13}	0.6232	0.4432	0.2422	0.1105	0.0891	0.0868	0.0868
F_{22}	0.01601	0.10080	0.26972	0.42124	0.44738	0.45388	0.4555
F_{24}	0.9334	0.6866	0.3463	0.0871	0.0412	0.0327	0.0310

Table IX

RESULTS FOR STANDARD II AND E_R = 0.675 (E_M = 1.35)

Case No.	550	551	552	553	554	589	516
$B_3 = 10^{-5}$ B_4 =	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}
F_{11}	0.30916	0.32088	0.34703	0.37357	0.37578		0.37599
F_{12}	0.02862	0.14513	0.31251	0.45098	0.48198		0.48523
F_{13}	0.6622	0.5340	0.3405	0.1755	0.1422		0.1388
F_{22}	0.00869	0.06321	0.21220	0.39945	0.44012		0.45411
F_{24}	0.9627	0.7917	0.4753	0.1496	0.0779		0.0607

Case No.	555	556	557	558	554	559	517
$B_4 = 10^{-5}$ B_3 =	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}
F_{11}	0.01508	0.08864	0.21464	0.33913	0.37578		0.40493
F_{12}	0.02874	0.14462	0.30713	0.44916	0.48198		0.48540
F_{13}	0.9562	0.7667	0.4782	0.2117	0.1422		0.1097
F_{22}	0.253	0.29279	0.36365	0.43152	0.44012		0.44039
F_{24}	0.7183	0.5626	0.3292	0.1193	0.0779		0.0742

Case No.	585	586	587	588	554	584	515	515A
$B_3 = B_4$ =	10	1	10^{-1}	10^{-3}	10^{-5}	10^{-7}	10^{-10}	10^{-15}
F_{11}	0.01508	0.08831	0.21340	0.33863	0.37578		0.40664	0.41845
F_{12}	0.01542	0.09873	0.26614	0.44017	0.48198		0.50865	0.51636
F_{13}	0.9695	0.8130	0.5205	0.2212	0.1422		0.0847	0.0652
F_{22}	0.00868	0.06245	0.20730	0.39793	0.44012		0.46086	0.46532
F_{24}	0.9759	0.8388	0.5266	0.1619	0.0779		0.0305	0.0183

Table X

RESULTS FOR STANDARD II AND E_R = 0.3535 (E_M = 0.707)

Case No.	560	561	562	563	564	504	518
$B_3 = 10^{-5}$ B_4 =	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}
F_{11}	0.28622	0.29286	0.31130	0.33540	0.33788		0.33807
F_{12}	0.01569	0.09153	0.23386	0.39338	0.43833		0.44321
F_{13}	0.6981	0.6156	0.4548	0.2712	0.2238		0.2187
F_{22}	0.00464	0.03724	0.15283	0.36163	0.42189		0.44632
F_{24}	0.9797	0.8712	0.6133	0.2450	0.1398		0.1105

Case No.	565	566	567	568	564	569	519
$B_4 = 10^{-5}$ B_3 =	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}
F_{11}	0.00810	0.05315	0.15280	0.28750	0.33788		0.38250
F_{12}	0.01573	0.09126	0.22971	0.39111	0.43833		0.44359
F_{13}	0.9762	0.8556	0.6175	0.3214	0.2238		0.1739
F_{22}	0.24639	0.27445	0.33569	0.41043	0.42189		0.42225
F_{24}	0.7379	0.6343	0.4346	0.1985	0.1398		0.1342

Case No.	500	501	502	503	564	513	514	529
$B_4 = B_3$ =	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}	10^{-15}
F_{11}	0.00810	0.05306	0.15215	0.28708	0.33788		0.38495	0.40411
F_{12}	0.00826	0.05892	0.19047	0.37904	0.43833		0.48157	0.49513
F_{13}	0.9836	0.8880	0.6574	0.3339	0.2238		0.1335	0.1008
F_{22}	0.00464	0.03698	0.14996	0.35999	0.42189		0.45748	0.46596
F_{24}	0.9871	0.9041	0.6596	0.2610	0.1398		0.0610	0.0389

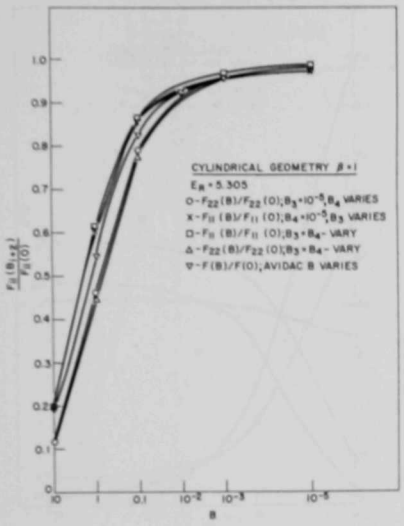
Table XI

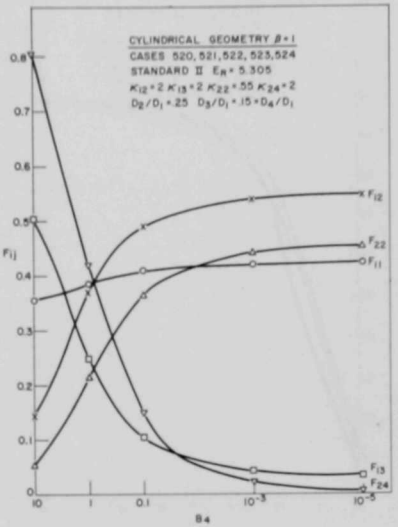
RESULTS FOR STANDARD II AND E_R = 0.1875 (E_M = 0.375)

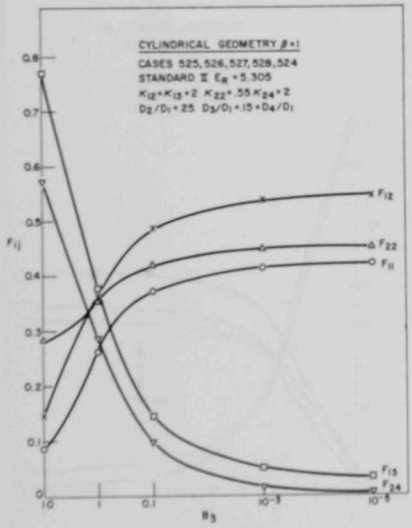
Case No.	570	571	572	573	574	595	596	597
$B_3 = 10^{-5}$ B_4 =	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}	10^{-15}
F_{11}	0.25275	0.25595	0.26637	0.28365	0.28590	0.28597		0.28605
F_{12}	0.00853	0.05458	0.16093	0.32126	0.37912	0.38558		0.38579
F_{13}	0.7387	0.6895	0.5727	0.3951	0.3350	0.3285		0.3282
F_{22}	0.00249	0.02118	0.10130	0.30567	0.38629	0.4156		0.43026
F_{24}	0.9890	0.9242	0.7378	0.3731	0.2346	0.1988		0.1840

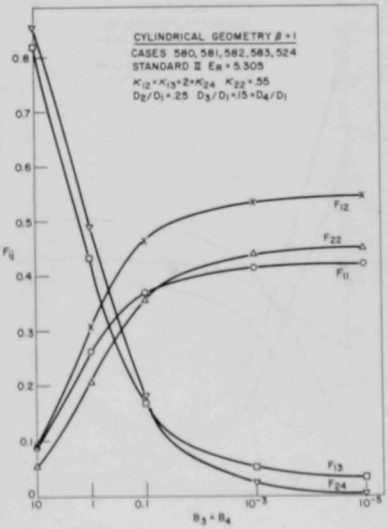
Case No.	575	576	577	578	574	594	598	599
$B_4 = 10^{-5}$ B_3 =	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}	10^{-15}
F_{11}	0.00436	0.03055	0.10035	0.22601	0.28590			0.36987
F_{12}	0.00854	0.05447	0.15836	0.31895	0.37912			0.38638
F_{13}	0.9871	0.9150	0.7413	0.4550	0.3350			0.2438
F_{22}	0.23493	0.25395	0.30141	0.37313	0.38629			0.38672
F_{24}	0.7565	0.6916	0.5402	0.3079	0.2346			0.2269

Case No.	590	591	592	593	574		579	512
$B_3 = B_4$ =	10	1	0.1	10^{-3}	10^{-5}		10^{-10}	10^{-15}
F_{11}	0.00436	0.03053	0.10010	0.22572	0.28590		0.3497	0.3779
F_{12}	0.00444	0.03377	0.12582	0.30462	0.37912		0.4432	0.4655
F_{13}	0.9912	0.9357	0.7741	0.4697	0.3350		0.2071	0.1566
F_{22}	0.00249	0.02110	0.09993	0.30421	0.38629		0.4437	0.4574
F_{24}	0.9931	0.9451	0.7743	0.3912	0.2346		0.1131	0.0771

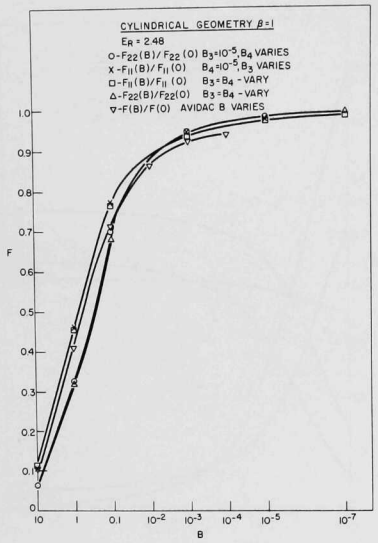


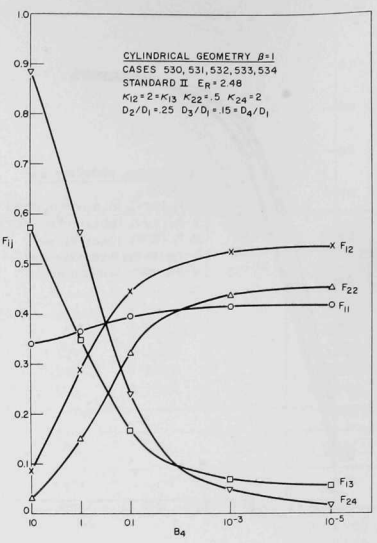


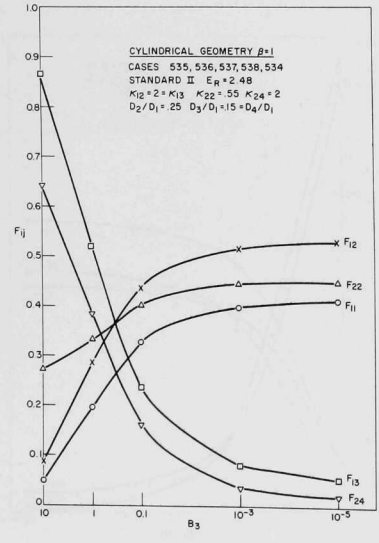


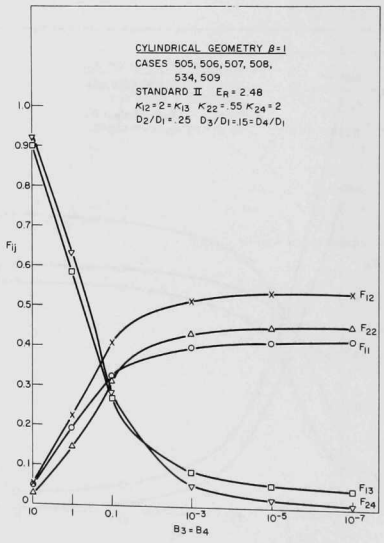


Figs. 1-4. Dependence of Normalized Recombination Fractions on B_i (E = 5.305)

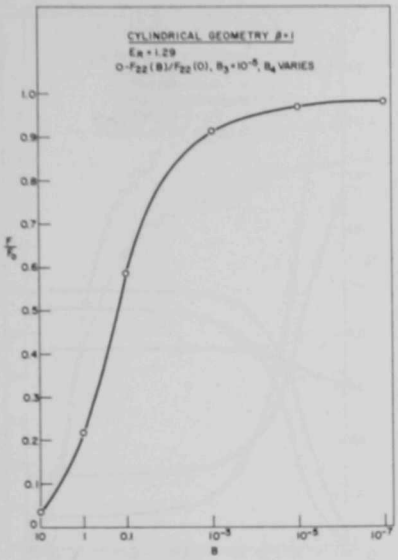


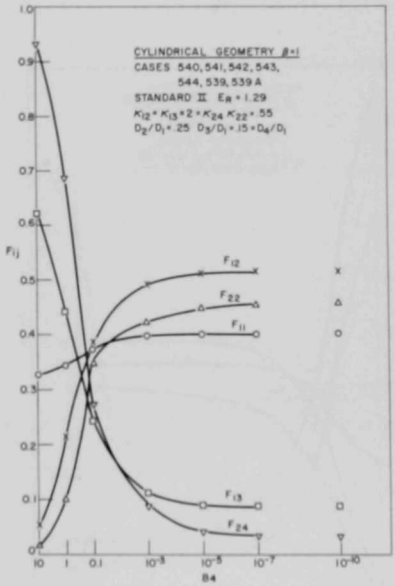




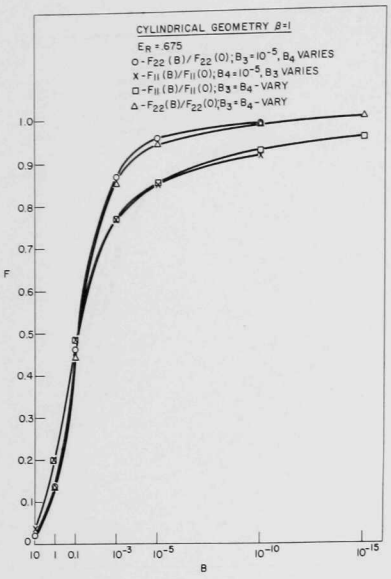


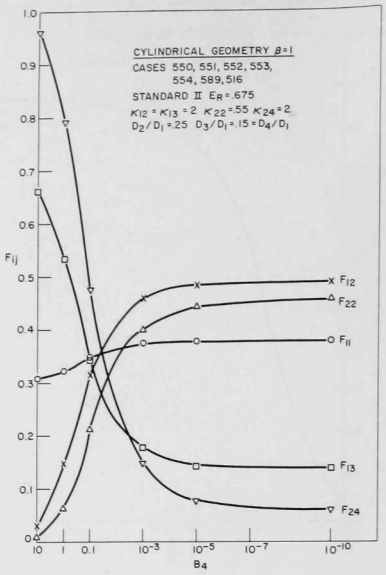
Figs. 5-8. Dependence of Normalized Recombination Fractions on B_i (E = 2.48)

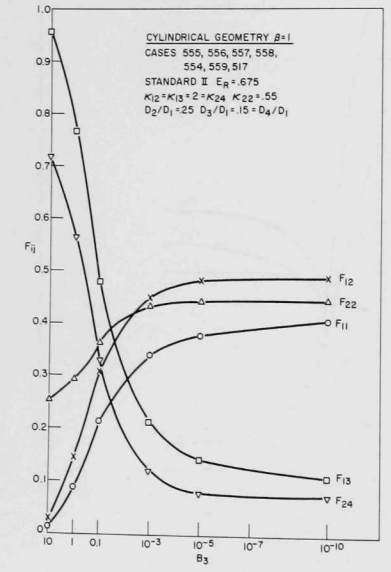


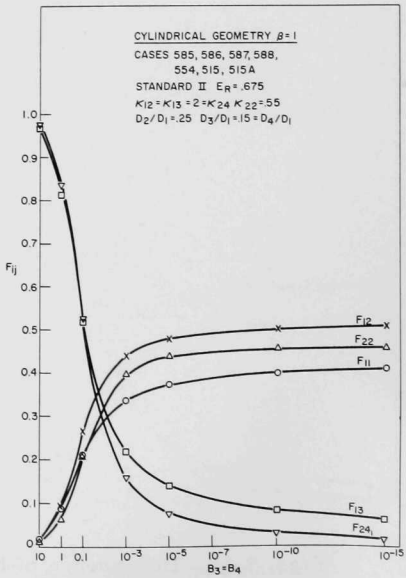


Figs. 9-10. Dependence of Normalized Recombination Fractions on B_i (E = 1.29)

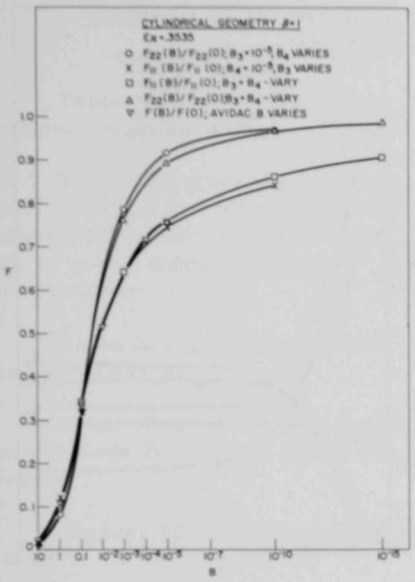


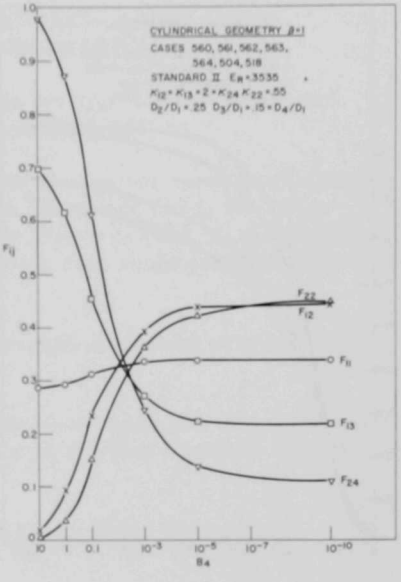


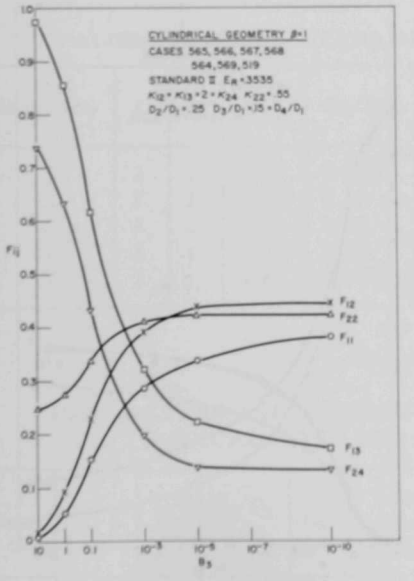


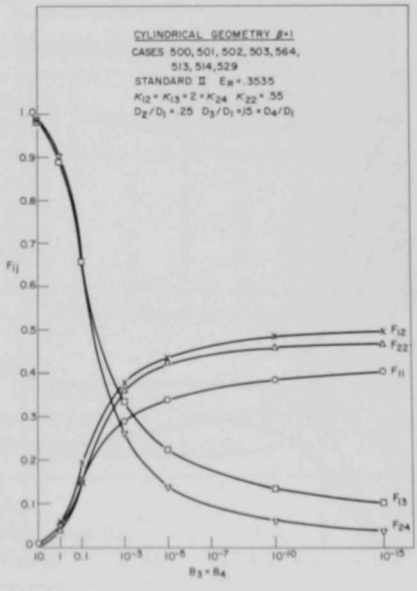


Figs. 11-14. Dependence of Normalized Recombination Fractions on B_i (E = 0.675)

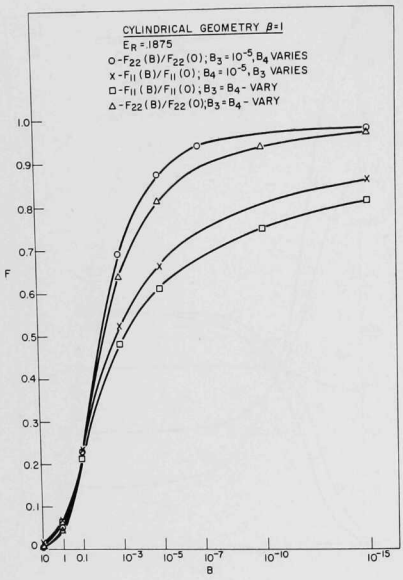


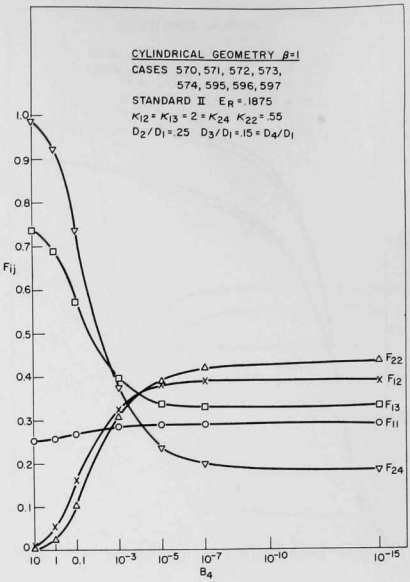


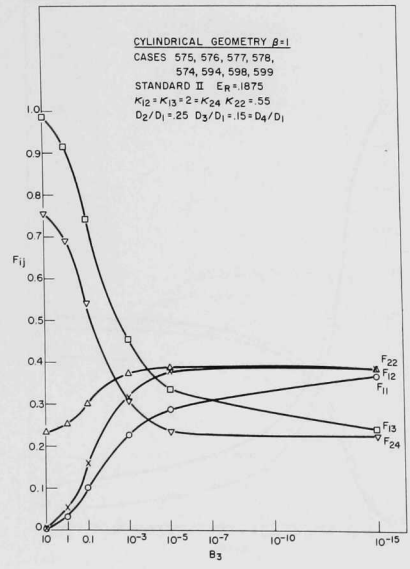


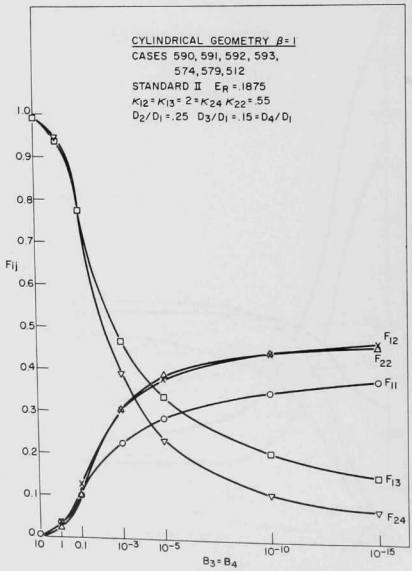


Figs. 15-18. Dependence of Normalized Recombination Fractions on B_i (E = 0.3535)









Figs. 19-22. Dependence of Normalized Recombination Fractions on B_i (E = 0.1875)

SECTION TWO: FINAL RESULTS FOR γ-RAY CASES (SPHERICAL GEOMETRY)

Table XII gives the standard values for five sets of parameter combinations which were investigated most thoroughly.

Table XIII gives values of parameters used for some preliminary spherical cases limited to one radical and one solute (Code B). Comparisons were made with previous runs by Flanders (Ref. 2) and Phillips (Ref. 3) on the Avidac and George, with codes that could accommodate only two reactions.

Table XIV gives parameters and results for cases with two radicals only (Code A).

Table XV gives results for the spherical cases run with four components (Code B), most of which are based on the five standard sets of values.

Figures 23-35 are graphs of final F_{ij} vs B for the cases in Table XV.

Table XII

VALUES OF PARAMETERS FOR STANDARD γ-RAY CASES

Standard	ϵ	β	E	D_2/D_1	D_4/D_1 D_3/D_1	k_{12}/k_{11}	k_{24}/k_{11} k_{13}/k_{11}	k_{22}/k_{11}
I	2	1	0.87	0.4545	0.15	2	2	1
II	2	1	0.87	0.25	0.15	2	2	0.55
III	2	1	0.91	0.25	0.15	4	2	0.60
IV	2	1	0.87	0.25	0.15	1	2	0.55
V	2	1	0.87	0.125	0.15	2	2	0.30

Table XIII

PARAMETERS AND RESULTS FOR CASES WITH ONLY ONE RADICAL (WITH AND WITHOUT A SOLUTE)

Case	ϵ	β	E	D_4/D_1 D_2/D_1	D_3/D_1	k_{24}/k_{11} k_{22}/k_{11} k_{12}/k_{11}	k_{13}/k_{11}	T_f	F_{11}	F_{13} or F_{10}
DP	2	1	2.5	0	1	0	1	0.17	0.1505	0.8495
DAF	2	1	2.5	0	0	0	0	0.05	0.430	0.570

Table XIV

SPHERICAL CASES WITH TWO COMPONENTS ONLY

β	Case No.	E	D_2/D_1	k_{12}/k_{11}	k_{22}/k_{11}	F_{11}	F_{12}	F_{22}	F_{10}	F_{20}	R_1	R_2
1	2-1	1.8	0.3333	2	1	0.2477	0.2999	0.4238	0.4525	0.2764	1.711	1.086
1	2-2	1.8	0.5	2	1	0.2503	0.2939	0.3697	0.4558	0.3365	1.477	1.278
1	2-3	1.8	0.6667	2	1	0.2539	0.2858	0.3302	0.4603	0.3840	1.300	1.445
1	2-4	1.8	1	2	1	0.2615	0.2615	0.2615	0.4771	0.4771	1.000	1.825
1	2-5	2.5	0.3333	2	1	0.2810	0.3317	0.4485	0.3873	0.2198	1.596	0.832
1	2-6	2.5	0.5	2	1	0.2846	0.3279	0.4016	0.3876	0.2705	1.411	0.959
1	2-7	2.5	0.6667	2	1	0.2886	0.3208	0.3649	0.3907	0.3143	1.265	1.079
1	2-8	2.5	1	2	1	0.2972	0.2972	0.2972	0.4056	0.4056	1.000	1.365
1	2-9	3.2	0.3333	2	1	0.3053	0.3543	0.4641	0.3404	0.1816	1.520	0.678
1	2-10	3.2	0.5	2	1	0.3089	0.3513	0.4221	0.3398	0.2267	1.366	0.775
1	2-11	3.2	0.6667	2	1	0.3131	0.3448	0.3879	0.3420	0.2672	1.239	0.869
1	2-12	3.2	1	2	1	0.3224	0.3224	0.3224	0.3552	0.3552	1.000	1.102
1	1	1.25	0.3333	2	1	0.2094	0.2604	0.3861	0.5302	0.3535	1.844	1.484
1	2	1.25	0.5	2	1	0.2114	0.2535	0.3285	0.5352	0.4180	1.554	1.766
1	3	1.25	0.6667	2	1	0.2144	0.2441	0.2875	0.5410	0.4678	1.341	2.010
1	4	1.25	1	2	1	0.2201	0.2201	0.2201	0.5599	0.5599	1.000	2.544
1	5	0.6	0.333	2	1	0.1365	0.1803	0.2948	0.6832	0.5249	2.160	2.801
1	6	0.6	0.5	2	1	0.1381	0.1714	0.2334	0.6905	0.5952	1.690	3.461
1	7	0.6	0.6667	2	1	0.1398	0.1623	0.1948	0.6979	0.6429	1.393	4.007
1	8	0.6	1	2	1	0.1423	0.1423	0.1423	0.7154	0.7154	1.000	5.027
1	10	0.8	0.45	2	1	0.1651	0.2053	0.2857	0.6296	0.5090	1.731	2.526
1	11	0.8	0.5	2	1	0.1658	0.2026	0.2701	0.6317	0.5273	1.629	2.659
1	251	0.87	0.4545	1.5	0.5	0.1812	0.1854	0.1943	0.6335	0.6204	1.072	3.340
2	252	0.87	0.4545	2	1	0.1659	0.2060	0.4384	0.6281	0.3556	2.642	1.628
1	253	0.87	0.4545	2	1	0.1737	0.2145	0.2951	0.6118	0.4904	1.699	2.351
2	254	0.87	0.25	1.3	0.3	0.1746	0.1860	0.2280	0.6394	0.5859	1.306	3.043
1	255	0.87	0.4545	2	1	0.1708	0.2236	0.3904	0.6056	0.3860	2.286	1.767
1	256	0.87	0.25	1.75	0.75	0.1776	0.2007	0.2511	0.6217	0.5482	1.413	2.729
1	257	0.87	0.25	2	0.55	0.1670	0.2412	0.2735	0.5918	0.4853	1.637	2.445
1	258	1.10	0.25	1.25	0.25	0.2102	0.2081	0.2004	0.5817	0.5915	0.953	2.857
1	259	0.75	0.25	3.125	1	0.1388	0.2871	0.3289	0.5741	0.3840	2.370	2.048
1	260	0.8	0.25	1	0.5	0.1814	0.1344	0.2874	0.6842	0.5782	1.584	2.693
1	261	0.8	0.25	2	0.5	0.1589	0.2331	0.2476	0.6080	0.5193	1.558	2.773
1	262	0.8	0.25	4	0.5	0.1282	0.3697	0.1938	0.5021	0.4365	1.512	2.915
1	263	0.89	0.25	2	0.53	0.1690	0.2450	0.2265	0.5860	0.4856	1.594	2.444
1	264	0.87	0.125	2	0.55	0.1651	0.2434	0.3264	0.5915	0.3810	2.274	1.798
1	265	0.87	0.25	1	0.55	0.1918	0.1397	0.3844	0.6685	0.5417	1.661	2.371
1	266	0.435	0.25	2	0.55	0.1073	0.1602	0.1416	0.7325	0.6456	1.810	4.902
1	267	0.87	0.25	2	0.275	0.1649	0.2558	0.0883	0.5793	0.5784	1.006	3.501
1	268	0.87	0.25	4	0.55	0.1337	0.3802	0.0759	0.4861	0.4107	1.564	2.615
1	269	0.87	0.5	2	0.55	0.1711	0.2265	0.1843	0.6024	0.5893	1.077	3.353
1	270	1.74	0.25	2	0.55	0.2340	0.3264	0.3426	0.4397	0.3310	1.465	1.337
1	271	0.91	0.25	4	0.6	0.1370	0.3844	0.2293	0.4787	0.3864	1.674	2.362
1	272	0.87	0.125	1	0.55	0.1879	0.1416	0.4381	0.6706	0.4203	2.332	1.743
1	273	0.435	0.25	1	0.55	0.1175	0.0883	0.2154	0.7942	0.6963	1.834	4.477
1	274	0.87	0.25	0.5	0.55	0.2075	0.0759	0.3473	0.7166	0.5768	1.674	2.331
1	275	0.87	0.25	1	0.275	0.1902	0.1499	0.1968	0.6599	0.6533	1.035	3.394
1	276	1.74	0.25	1	0.55	0.2827	0.1990	0.4192	0.5183	0.3818	1.483	1.282
1	279	0.75	0.125	2	0.275	0.1496	0.2414	0.2341	0.6090	0.5245	1.565	2.954
1	280	0.87	0.125	2	0.30	0.1629	0.2592	0.2633	0.5780	0.4775	1.616	2.476
0.5	281	0.87	0.25	2	0.275							
2	282	0.87	0.25	2	0.275	0.1531	0.2622	0.2808	0.5847	0.4571	1.834	2.401
1	283	0.87	0.25	2	1.10	0.1712	0.2199	0.4096	0.6089	0.3705	2.392	1.686
0.5	284	0.87	0.25	2	0.55							
2	285	0.87	0.25	2	0.55	0.1586	0.2335	0.4157	0.6079	0.3508	2.621	1.669

Table XV

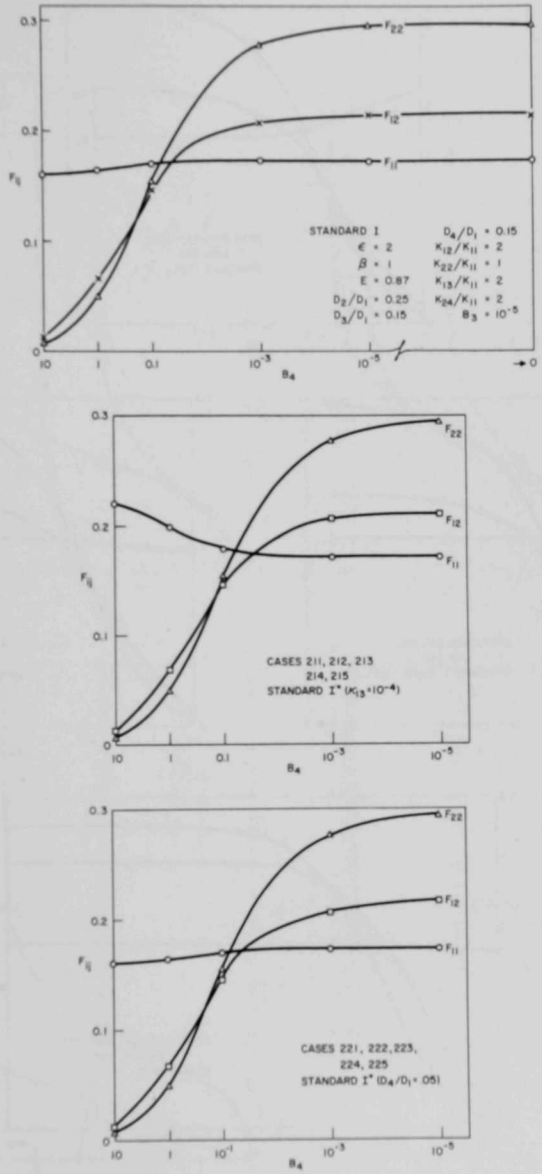
RESULTS FOR 4-COMPONENT γ-RAY CASES

Case No.	Deviation from Standard I			B_3 or B_4 Variable B	Calculated Concentrations & Corrected				
	E	D	Constant B		F_{11}	F_{12}	F_{22}	F_{13}	F_{24}
101	0.8	$D_2/D_1 = 0.4$	$B_4 = 10^{-5}$	$B_3 = 10^{-5}$	0.1629	0.2067	0.3031	0.6404	0.4902
102				10^{-3}	0.1557	0.1997	0.3026	0.6447	0.4977
103				10^{-1}	0.0989	0.1382	0.2879	0.7629	0.5738
104				1	0.0385	0.0626	0.2624	0.8990	0.6750
109				10	0.0062	0.0120	0.2452	0.9818	0.7428
105	0.1		$B_4 \geq 10^{-5}$	$B_3 \geq 10^{-5}$	0.1720	0.2134	0.2950	0.6146	0.4916
106				$\geq 10^{-3}$	0.1642	0.2059	0.2946	0.6299	0.4995
107				$\geq 10^{-1}$	0.1032	0.1415	0.2806	0.7553	0.5778
108				≥ 1	0.0394	0.0634	0.2567	0.8972	0.6798
110				≥ 10	0.0064	0.0121	0.2414	0.9815	0.7464
116		$D_2/D_1 = 1.0$	$B_3 \geq 10^{-5}$	$B_4 \geq 10^{-5}$	0.1794	0.1794	0.1794	0.6412	0.6412
117				$\geq 10^{-3}$	0.1793	0.1735	0.1708	0.6417	0.6557
118				$\geq 10^{-1}$	0.1755	0.1226	0.1056	0.7018	0.7718
119				≥ 1	0.1675	0.0579	0.0396	0.7745	0.9025
120				≥ 10	-	0.0118	0.0064	-	0.9818
105			$B_3 \geq 10^{-5}$	$B_4 \geq 10^{-5}$	0.1720	0.2134	0.2950	0.6146	0.4916
122				$\geq 10^{-3}$	0.1719	0.2061	0.2768	0.6219	0.5171
123				$\geq 10^{-1}$	0.1693	0.1428	0.1507	0.6878	0.7065
124				≥ 1	0.1640	0.0639	0.0470	0.7720	0.8891
125				≥ 10	0.1607	0.0121	0.0066	0.8271	0.9812
	Standard I Case								
141	E = 0.87 $D_2 = 0.4545$-- $D_3 = 0.15$ $D_4 = 0.15$	$K_{12} = 2$ $K_{13} = 2$ $K_{22} = 1$ $K_{24} = 2$	$B_3 = 10^{-5}$	$B_4 = 10^{-5}$	0.1720	0.2135	0.2951	0.6145	0.4915
142				10^{-3}	0.1720	0.2065	0.2776	0.6216	0.5160
143				10^{-1}	0.1695	0.1452	0.1547	0.6853	0.7001
144				1	0.1642	0.0668	0.0498	0.7690	0.8834
145				10	0.1603	0.0129	0.0070	0.8267	0.9800
	K	E	D	$B_3 = 10^{-5}$ Variable B_4					
151	$K_{13} = 10^{-2}$			10^{-5}	0.1718	0.2132	0.2947	0.6150	0.4921
152				10^{-3}	0.1720	0.2063	0.2772	0.6217	0.5164
153				10^{-1}	0.1792	0.1470	0.1547	0.6738	0.6984
154				1	0.1987	0.0681	0.0497	0.7331	0.8822
155				10	0.2185	0.0130	0.0070	0.7685	0.9800
203			$D_3/D_1 = 0.4545$--	10^{-5}	0.1720	0.2135	0.2951	0.6145	0.4914
202				10^{-1}	0.1709	0.1454	0.1547	0.6837	0.6998
201				10	0.1663	0.0129	0.0070	0.8207	0.9800
208			$D_4/D_1 = 0.4545$--	10^{-5}	0.1720	0.2135	0.2951	0.6145	0.4914
207				10^{-1}	0.1695	0.1448	0.1541	0.6856	0.7011
206				10	0.1603	0.0129	0.0070	0.8267	0.9800
211	$K_{13} = 10^{-4}$			10^{-5}	0.1720	0.2135	0.2951	0.6145	0.4914
212				10^{-3}	0.1722	0.2066	0.2776	0.6211	0.5158
213				10^{-1}	0.1795	0.1471	0.1548	0.6733	0.6980
214				1	0.1993	0.0682	0.0498	0.7325	0.8820
215				10	0.2197	0.0133	0.0072	0.7670	0.9796
216	$K_{13} = 10^{-2}$		$D_3/D_1 = 0$	10	-	0.0132	0.0072	-	-
221			$D_4/D_1 = 0.05$	10^{-5}	0.1720	0.2135	0.2951	0.6145	0.4915
222				10^{-3}	0.1728*	0.2063*	0.2760*	0.6208*	0.5177*
223				10^{-1}	0.1695	0.1453	0.1550	0.6851	0.6997
224				1	0.1642	0.0668	0.0498	0.7690	0.8833
225				10	0.1603	0.0129	0.0070	0.8267	0.9800
231	$K_{24} = 0.02$			10^{-5}	0.1720	0.2135	0.2951	0.6145	0.4915
232				10^{-3}	0.1720	0.2063	0.2770	0.6217	0.5167
233				10^{-1}	0.1694	0.1431	0.1507	0.6875	0.7061
234				1	0.1641	0.0654	0.0485	0.7704	0.8861
235				10	0.1603	0.0128	0.0070	0.8268	0.9802

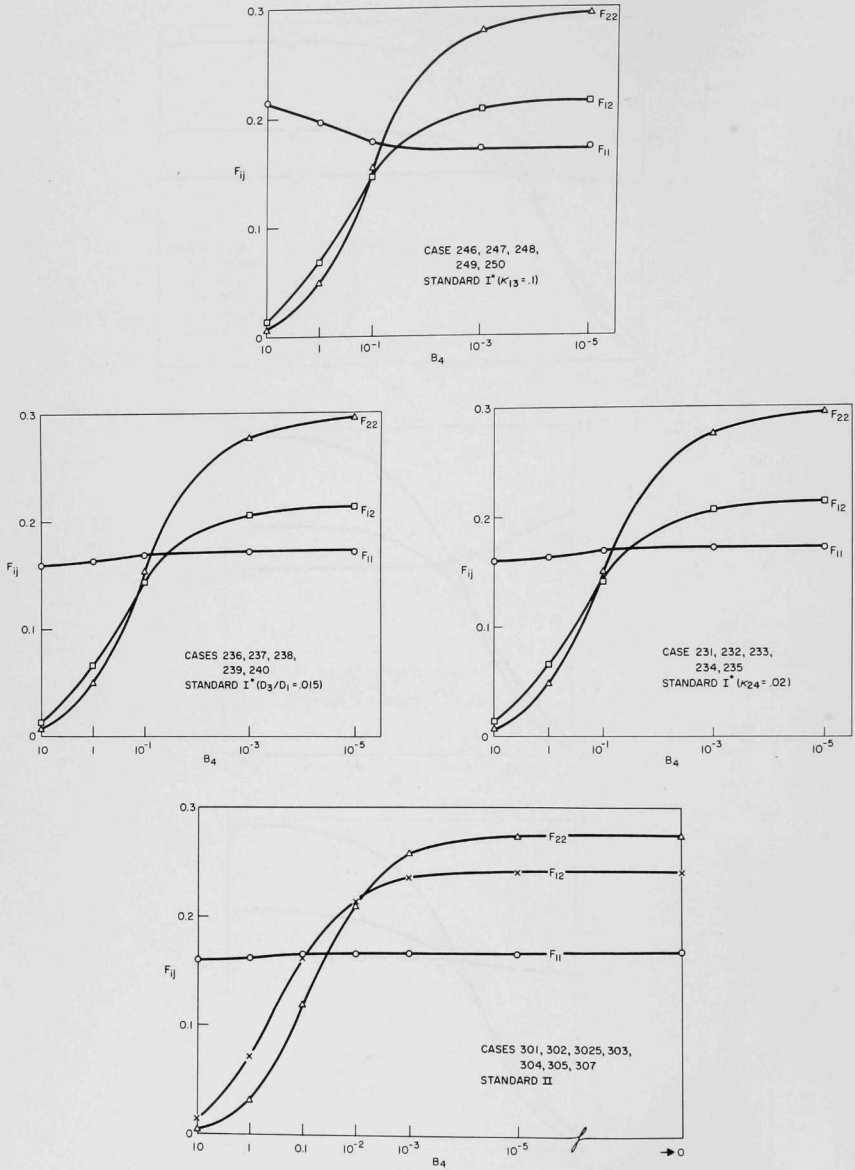
Table XV (Cont'd.)

Case No.	Deviation from Standard I			$B_3 = 10^{-5}$ Variable B_4	Calculated Concentrations & Corrected				
	K	E	D		F_{11}	F_{12}	F_{22}	F_{13}	F_{24}
236			$D_3/D_1 = 0.015$	10^{-5}	0.1720	0.2135	0.2951	0.6145	0.4914
237				10^{-3}	0.1720	0.2064	0.2776	0.6216	0.5160
238				10^{-1}	0.1690	0.1450	0.1547	0.6859	0.7003
239				1	0.1633	0.0667	0.0498	0.7699	0.8835
240				10	0.1591	0.0129	0.0070	0.8280	0.9800
246	$K_{13} = 0.1$			10^{-5}	0.1720	0.2135	0.2951	0.6145	0.4914
247				10^{-3}	0.1722	0.2066	0.2776	0.6211	0.5158
248				10^{-1}	0.1789	0.1470	0.1548	0.6740	0.6981
249				1	0.1969	0.0681	0.0498	0.7350	0.8820
250				10	0.2149	0.0130	0.0070	0.7720	0.9799
	D_2/D_1	K_{12} K_{22}	E	B	Extrapolated Concentrations and By Difference				
Std. II	0.25	2 0.55	0.87	$B_3 = 10^{-5}$					
301				$B_4 = 10^{-5}$	0.1667	0.2405	0.2731	0.5928	0.4864
302				10^{-3}	0.1666	0.2356	0.2575	0.5978	0.5169
3025				10^{-2}	0.1663	0.2141	0.2092	0.6196	0.5767
303				0.1	0.1650	0.1617	0.1196	0.6733	0.7187
304				1	0.1620	0.0712	0.0312	0.7668	0.8976
305				10	0.1600	0.0132	0.0040	0.8268	0.9829
Std. III	0.25	4 0.60	0.91	$B_3 = 10^{-5}$					
311				$B_4 = 10^{-5}$					
312				10^{-3}	0.1368	0.3769	0.2170	0.4864	0.4061
3125				10^{-2}	0.1374	0.3480	0.1799	0.5146	0.4721
313				0.1	0.1404	0.2743	0.1080	0.5853	0.6177
314				1	0.1500	0.1324	0.0317	0.7176	0.8359
315				10					
Std. IV	0.25	1 0.55	0.87	$B_3 = 10^{-5}$					
316				$B_4 = 10^{-5}$					
317				10^{-3}	0.1912	0.1361	0.2993	0.6727	0.5646
3175				10^{-2}	0.1899	0.1225	0.2406	0.6876	0.6365
318				0.1	0.1841	0.0902	0.1345	0.7357	0.7753
319				1	0.1711	0.0377	0.0331	0.7912	0.9292
320				10					
Std. V	0.125	2 0.30	0.87	$B_3 = 10^{-5}$					
306				$B_4 = 10^{-5}$	0.1625	0.2585	0.2657	0.5790	0.4759
307				10^{-3}	0.1625	0.2539	0.2470	0.5836	0.4991
3075				10^{-2}	0.1624	0.2313	0.1862	0.6063	0.5825
308				0.1	0.1616	0.1740	0.0902	0.6645	0.7359
309				1	0.1603	0.0743	0.0187	0.7655	0.9070
310				10	0.1597	0.0133	0.0022	0.8270	0.9875
Std. II*	0.25	2 0.55	0.87	$B_3 = B_4$					
301				$B_4 = 10^{-5}$	0.1667	0.2405	0.2731	0.5928	0.4864
321				10^{-3}	0.1610	0.2313	0.2571	0.6074	0.5116
322				10^{-2}	0.1435	0.2018	0.2081	0.6547	0.5901
323				0.1	0.1032	0.1361	0.1180	0.7607	0.7459
324				1	0.0412	0.0472	0.0310	0.9117	0.9218
325				10	0.0068	0.0070	0.0040	0.9863	0.9891
		K	D	$B_3 = 10^{-5}$ Variable B_4	Calculated Concentrations & Corrected				
400		$k_{13}/k_{11} = 0.1$	$D_3/D_1 = 0.015$	10	0.2160	0.0132	0.0072	0.0771	0.0980
401				1	0.1981	0.0683	0.0500	0.734	0.882
402				0.1	0.1800	0.1473	0.1551	0.673	0.698
403				10^{-3}	0.1730	0.209	0.280	0.618	0.511
404									
405		$k_{13}/k_{11} = 0.5$		10	0.2010	0.0132	0.0072	0.786	0.980
406				1	0.1893	0.0680	0.0500	0.743	0.882
407				0.1	0.1777	0.1469	0.1550	0.675	0.698
408				10^{-3}	0.1730	0.2068	0.2778	0.620	0.515
409									
	Deviation from Standard III								
271A				1	0.1798	0.1351	0.0317	0.685	0.833
271B				10	0.2170	0.0269	0.0044	0.756	0.969
271C				0.1	0.1474	0.2778	0.1080	0.575	0.614

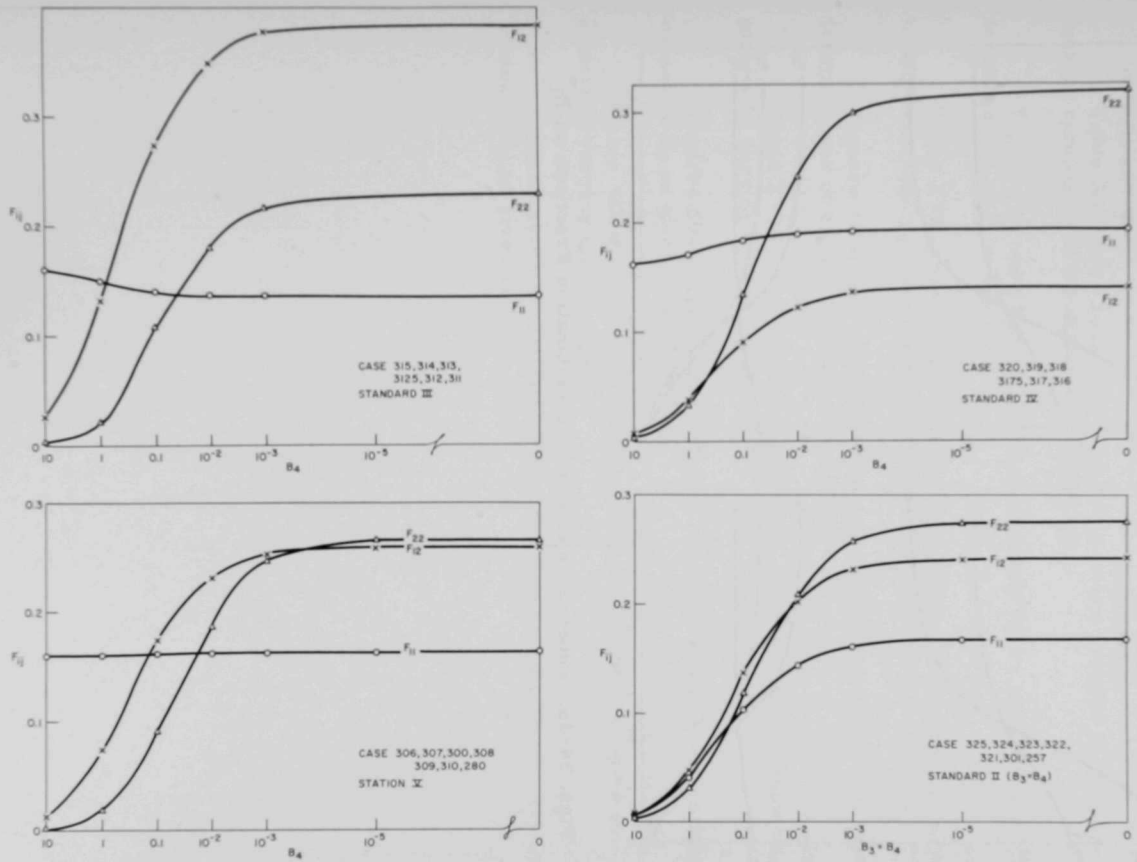
*55 points instead of the usual 33.



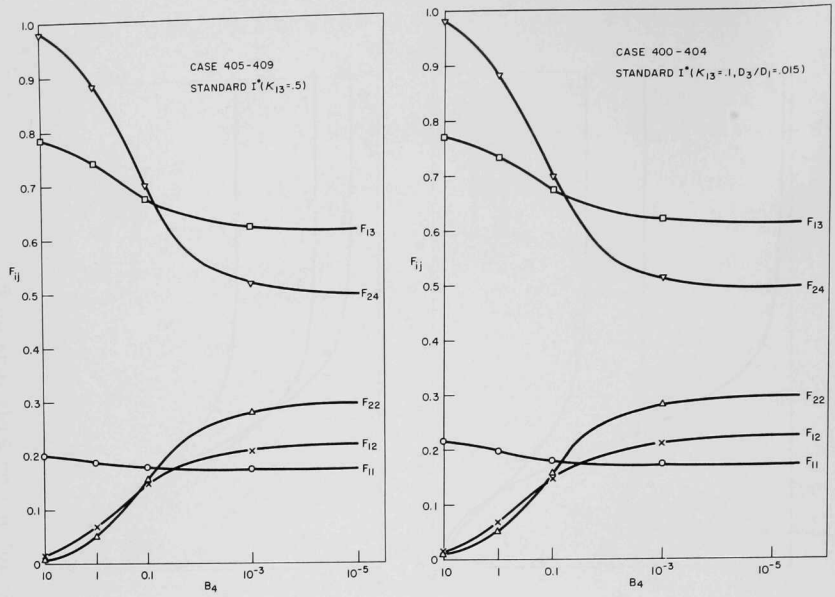
Figs. 23-25. Dependence of Final Recombination Fractions on B_i.



Figs. 26-29. Dependence of Final Recombination Fractions on B_i.



Figs. 30-33. Dependence of Final Recombination Fractions on B_i.



Figs. 34-35. Dependence of Final Recombination Fractions on B_i.

SECTION THREE: INFLUENCE OF PARAMETERS ON RESULTS FOR α-RAY AND γ-RAY CASES

Table XVI gives results of cylindrical cases grouped to facilitate making comparisons for different values of E.

Figures 36 and 37 are plots of normalized F_{ii} vs. B_{i+2} for the different values of E in Table XVI.

Table XVII gives results of the Standard Spherical cases, grouped to facilitate making comparisons for different values of κ_{12} and D_2/D_1.

Figures 38 and 39 are plots of normalized F_{22} vs. B_4 for the different values of κ_{12} and D_2/D_1 in Table XVII.

Table XVIII gives results of spherical cases grouped to show the effects of varying κ_{13} and D_3/D_1.

Figures 40-43 are graphs of F_{ij} vs. B_4, κ_{13}, or D_3/D_1 for certain values of B_4 as given in Table XVIII.

Table XIX gives results of spherical cases grouped to show the effects of varying κ_{24} and D_4/D_1.

Figures 44-45 are graphs of F_{ij} vs. B_4, κ_{24}, or D_4/D_1 for certain values of B_4 as given in Table XIX.

Table XVI

RESULTS OF CYLINDRICAL CASES FOR DIFFERENT VALUES OF E TO PLOT NORMALIZED F'S VS. B

Case No.	E	$B_3 = 10^{-5}$, $B_4 =$	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}	0*
520··	5.305	F_{22}	0.0530	0.2126	0.3625	0.4397	0.4505			0.46
		$F_{22}/F(0)$	0.115	0.462	0.788	0.956	0.979			1
	(10.61)	1-Avidac	0.190	0.547	0.824	0.957				1
530··	2.48	F_{22}	0.0289	0.1493	0.3191	0.4329	0.4494			0.46
		$F_{22}/F(0)$	0.063	0.325	0.694	0.941	0.977			1
	(4.96)	1-Avidac	0.101	0.411	0.715	0.923				1
540··	1.29	F_{22}	0.0160	0.1008	0.2697	0.4212	0.4474	0.4539	0.4555	0.46
		$F_{22}/F(0)$	0.035	0.219	0.586	0.916	0.973	0.987	0.990	1
	(2.58)	1-Avidac								1
550··	0.675	F_{22}	0.0087	0.0632	0.2122	0.3995	0.4401		0.4541	0.46
		$F_{22}/F(0)$	0.019	0.137	0.462	0.869	0.957		0.988	1
	(1.35)	1-Avidac								1
560··	0.3535	F_{22}	0.0046	0.0372	0.1528	0.3616	0.4219		0.4463	0.46
		$F_{22}/F(0)$	0.010	0.081	0.332	0.787	0.918		0.971	1
	(0.707)	1-Avidac	0.020	0.110	0.320	0.643	0.760	0.833		1
570··	0.1875	F_{22}	0.0025	0.0212	0.1013	0.3057	0.3863	10^{-10}	10^{-15}	0.46
		$F_{22}/F(0)$	0.005	0.046	0.220	0.665	0.840	0.4156	0.4303	1
	(0.375)	1-Avidac						0.903	0.935	
	(0.0707)	1-Avidac		0.012				0.337		1
Case No.	E	$B_4 = 10^{-5}$, $B_3 =$	10	1	0.1	10^{-3}	10^{-5}	10^{-7}	10^{-10}	0*
525··	5.305	F_{11}	0.0859	0.2619	0.3712	0.4137	0.4213			0.425
		$F_{11}/F(0)$	0.202	0.616	0.873	0.973	0.991			1
535··	2.48	F_{11}	0.0487	0.1960	0.3279	0.3992	0.4128			0.425
		$F_{11}/F(0)$	0.115	0.462	0.772	0.940	0.972			1
545··	1.29	F_{11}								
		$F_{11}/F(0)$								
555··	0.675	F_{11}	0.0151	0.0886	0.2146	0.3391	0.3758		0.4049	0.425
		$F_{11}/F(0)$	0.036	0.208	0.505	0.798	0.884		0.953	1
565··	0.3535	F_{11}	0.0081	0.0532	0.1528	0.2875	0.3379		0.3825	0.425
		$F_{11}/F(0)$	0.019	0.116	0.360	0.676	0.795		0.900	1
575··	0.1875	F_{11}	0.0044	0.0306	0.1004	0.2260	0.2859		10^{-15}	0.425
		$F_{11}/F(0)$	0.010	0.072	0.236	0.532	0.673		0.3699	1
									0.870	

*Rough extrapolated values.

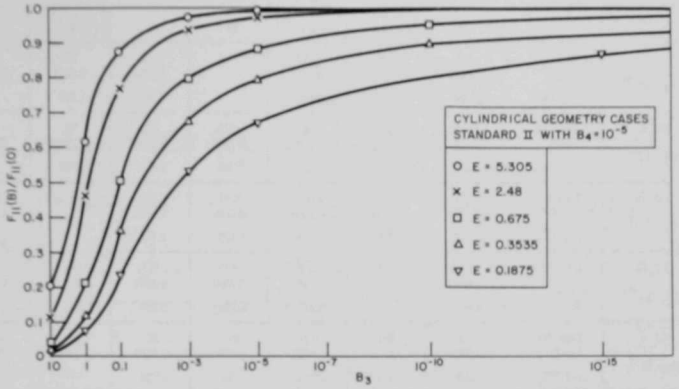


Fig. 36. Influence of Initial Free Radical Concentrations on $F_{11}(B)/F_{11}(0)$

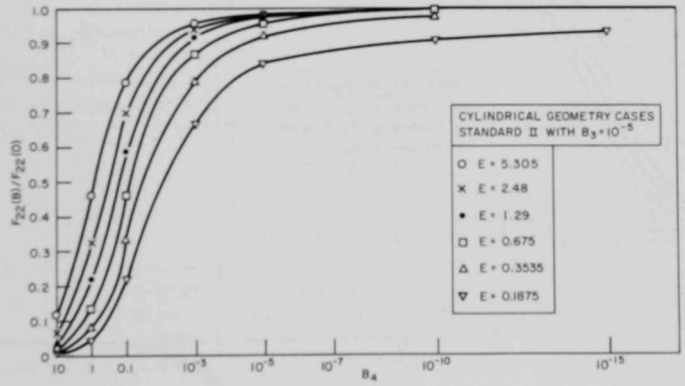


Fig. 37. Influence of Initial Free Radical Concentrations on $F_{22}(B)/F_{22}(0)$

Table XVII

RESULTS OF STANDARD CASES WITH SPHERICAL SYMMETRY

	B_4	10	1	0.1	10^{-2}	10^{-3}	10^{-5}	0
Std. I	Case No.	145	144	143	-	142	141	253
$B_3 = 10^{-5}$	$F_{22}(B)$	0.0070	0.0498	0.1547		0.2776	0.2951	0.2951
	$F(B)/F(0)$	0.024	0.169	0.524		0.941	1.000	1
Std. II	Case No.	305	304	303	3025	302	301	257
$B_3 = 10^{-5}$	$F_{22}(B)$	0.0039	0.0312	0.1195	0.2092	0.2575	0.2713	0.2735
	$F(B)/F(0)$	0.014	0.114	0.437	0.765	0.941	0.992	1
Std. III	Case No.	315	314	313	3125	312	311	271
$B_3 = 10^{-5}$	$F_{22}(B)$	0.0044	0.0317	0.1080	0.1799	0.2170	-	0.2293
	$F(B)/F(0)$	0.020	0.138	0.471	0.785	0.946		1
Std. IV	Case No.	320	319	318	3175	317	316	265
$B_3 = 10^{-5}$	$F_{22}(B)$	0.0040	0.0331	0.1345	0.2409	0.2993	-	0.3186
	$F(B)/F(0)$	0.029	0.104	0.422	0.756	0.939		1
Std. V	Case No.	310	309	308	3075	307	306	280
$B_3 = 10^{-5}$	$F_{22}(B)$	0.0022	0.0187	0.0902	0.1862	0.2470	0.2657	0.2633
	$F(B)/F(0)$	0.008	0.071	0.343	0.707	0.938	1	1
Std. II*	Case No.	325	324	323	322	321	301	257
	$F_{11}(B)$	0.0068	0.0412	0.1032	0.1435	0.1610	0.1667	0.1670
$B_3 = B_4$	$F_{11}(B)/F(0)$	0.041	0.247	0.618	0.859	0.964	0.998	1
	$F_{22}(B)$	0.0040	0.0310	0.1180	0.2081	0.2571	0.2731	0.2735
	$F_{22}(B)/F(0)$	0.014	0.113	0.431	0.761	0.940	0.999	1

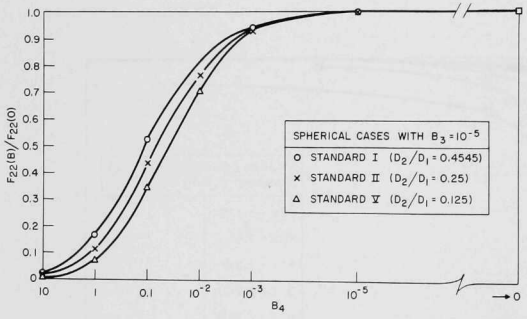


Fig. 38

Influence of Diffusion Coefficients on $F_{22}(B)/F_{22}(0)$

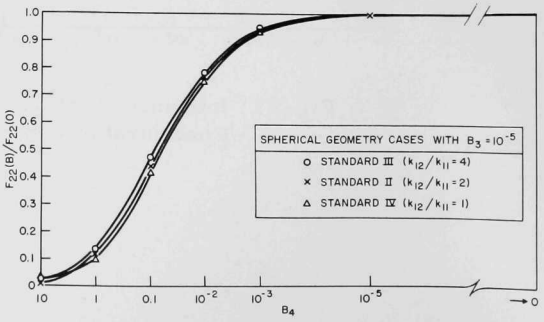


Fig. 39

Influence of Reaction Rates on $F_{22}(B)/F_{22}(0)$

Table XVIII

RESULTS WHEN k_{13}/k_{11} AND D_3/D_1 VARY FOR γ-RAY CASES

Case No.	Deviation from Std. I κ_{13}	D_3/D_1		Final Values of F_{11} @ B_4				
				10^{-5}	10^{-3}	10^{-1}	1	10
141-145	2.0		Std. I	0.1720	0.1720	0.1695	0.1642	0.1603
405-409	0.5				0.1730	0.1777	0.1893	0.2010
246-250	0.1			0.1720	0.1722	0.1789	0.1969	0.2149
151-155	10^{-2}			0.1718	0.1720	0.1792	0.1987	0.2185
211-215	10^{-4}			0.1720	0.1720	0.1795	0.1993	0.2197
203-201		0.4545··		0.1720	-	0.1709	-	0.1663
141-145		0.15	Std. I	0.1720	0.1720	0.1695	0.1642	0.1603
236-240		0.015		0.1720	0.1720	0.1690	0.1633	0.1591

Case No.	Deviation from Std. I κ_{13}	D_3/D_1		Final Values for B_4 = 10				
				F_{11}	F_{12}	F_{22}	F_{13}	F_{24}
145	2.0		Std. I	0.1603	0.0129	0.0070	0.8267	0.9800
405	0.5			0.2010	0.0132	0.0072	0.786	0.980
250	0.1			0.2149	0.0130	0.0070	0.7720	0.9799
155	10^{-2}			0.2185	0.0130	0.0070	0.7685	0.9800
215	10^{-4}			0.2197	0.0133	0.0072	0.7670	0.9796
201		0.4545··		0.1663	0.0129	0.0070	0.8207	0.9800
145		0.15	Std. I	0.1603	0.0129	0.0070	0.8267	0.9800
240		0.015		0.1591	0.0129	0.0070	0.8280	0.9800

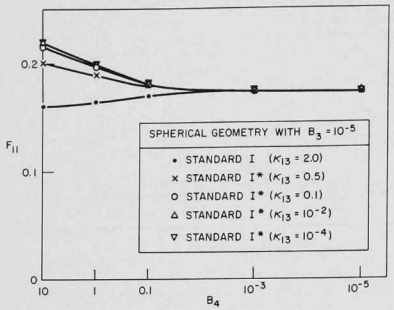


Fig. 40. Influence of Reaction Rates on F_{11}

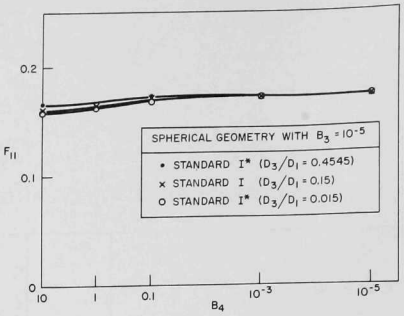


Fig. 41. Influence of Diffusion Rates on F_{11}

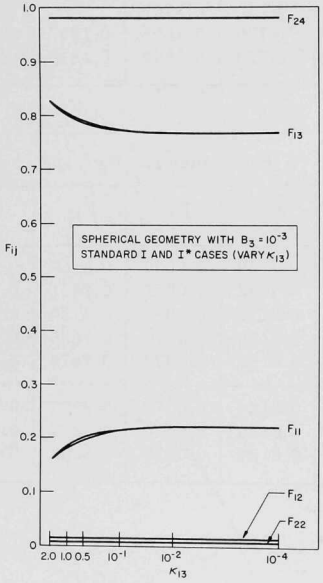


Fig. 42. Influence of Reaction Rate on F_{ij} for $B_4 = 10$

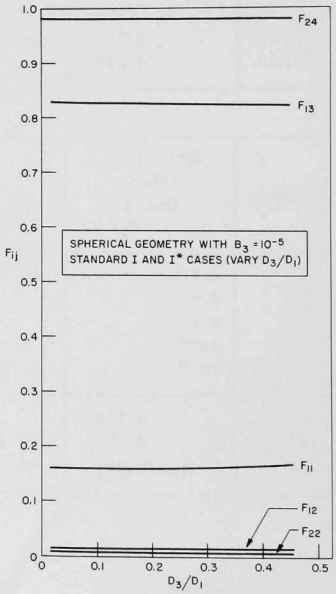


Fig. 43. Influence of Diffusion Rate on F_{ij} for $B_4 = 10$

Table XIX

RESULTS WHEN k_{24}/k_{11} AND D_4/D_1 VARY FOR γ-RAY CASES

Case No.	Deviation from Std.			Final Values of F_{22} @ B_4				
	κ_{24}	D_4/D_1		10^{-5}	10^{-3}	10^{-1}	1	10
141-145 231-235	2.0 0.02		Std.	0.2951 0.2951	0.2776 0.2770	0.1547 0.1507	0.0498 0.0485	0.0070 0.0072
206-206 141-145 221-225		0.4545-- 0.15 0.05	Std.	0.2951 0.2951 0.2951	- 0.2776 0.2760	0.1541 0.1547 0.1550	- 0.0498 0.0498	0.0070 0.0070 0.0070

Case No.	Deviation from Std.			Final Values for B_4 = 10				
	κ_{24}	D_4/D_1		F_{11}	F_{12}	F_{22}	F_{13}	F_{24}
145 235	2.0 0.02		Std.	0.1603 0.1603	0.0129 0.0128	0.0070 0.0070	0.8267 0.8268	0.9800 0.9802
206 145 225		0.4545-- 0.15 0.05	Std.	0.1603 0.1603 0.1603	0.0129 0.0129 0.0129	0.0070 0.0070 0.0070	0.8267 0.8267 0.8267	0.9800 0.9800 0.9800

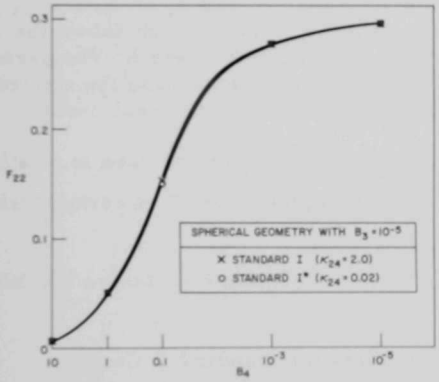


Fig. 44

Influence of Reaction Rate on F_{22}

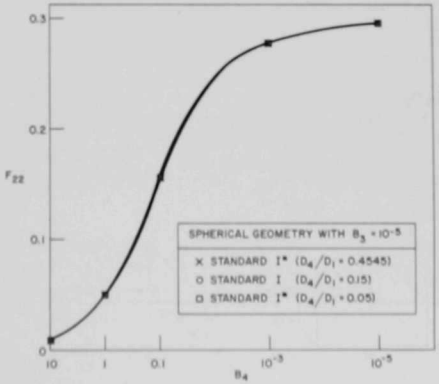


Fig. 45

Influence of Diffusion Rate on F_{22}

SECTION FOUR: FIGURES TRACING THE REACTIONS OVER TIME AND SPACE FOR γ-RAY CASES

As indicated previously, transformed time T goes from 1 to 0, while real time goes from 0 to ∞; and transformed space R goes from 1 to 0, so P goes from some integer at the origin down to 0, while the real space goes from 0 to ∞. All but Figure 46 are based on actual cases described in Table XV.

Figure 46: General shapes of solutions.

Figures 47-57: Graphs of the amounts of X_i (i=1,2,3,4) at the origin (center of initial concentration of free radicals) as a function of the real time plotted on a log scale. Figures 47-51 are for Standard I at different values of B_4, whereas Figures 52-57 are all for $B_4 = 1$ for different parameter combinations.

Figures 58-61: Similar plots for either X_1 and X_3 or X_2 and X_4 for $B_4 = 10$ only, with different cases grouped so each graph shows the influence of some parameter for cases similar to Standard I. The parameters being varied are D_3/D_1, κ_{13}, D_4/D_1, and κ_{24}; in each case the concentration of X_i at the origin is plotted against the log of the real time.

Tables XX to XXIII: Values of U_i $\left(i = \frac{1}{2}\middle|\frac{3}{4}\right)$ to be used in plotting U_i vs. T at certain values of R (or P) and to plot U_i vs. R at certain values of T for Standard II cases.

Figures 62-89: Plots based on the information in Tables XX-XXIII for the cases described in Table XV.

Figures 90 and 91 are similar plots for Standard V Cases.

Figures 92-103: Plots of F_{ij} vs. log t for Standard I cases and others with selected values of B_4.

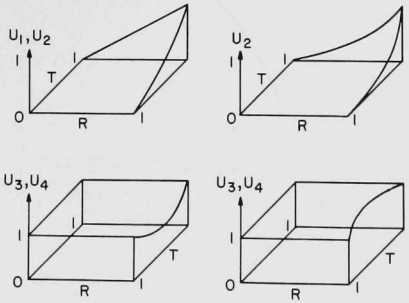
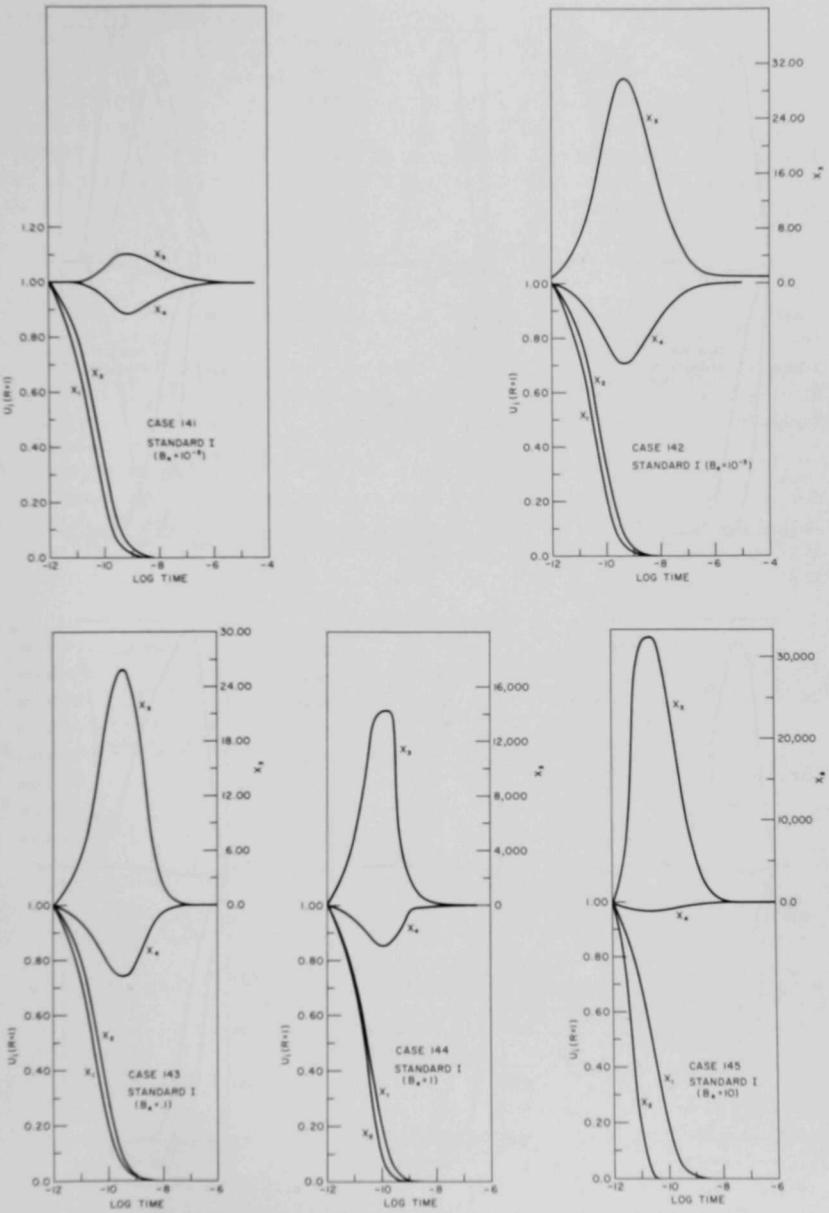
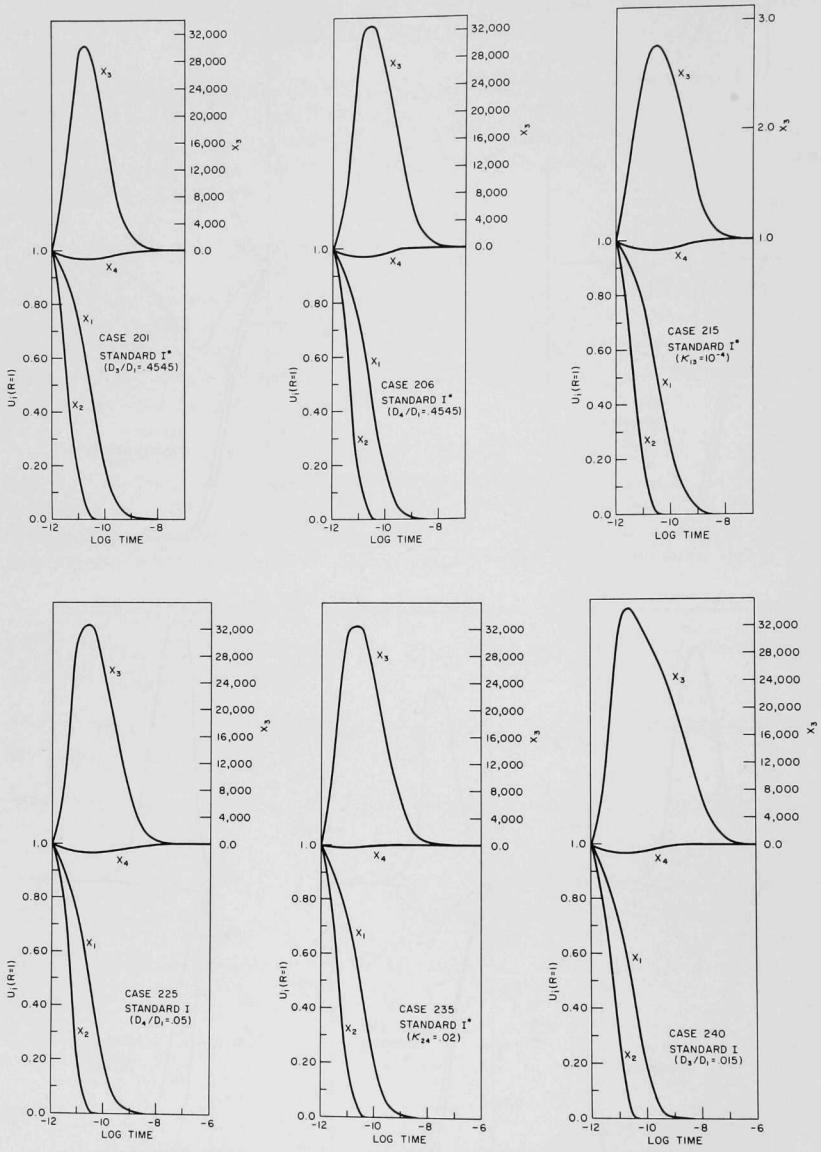


Fig. 46

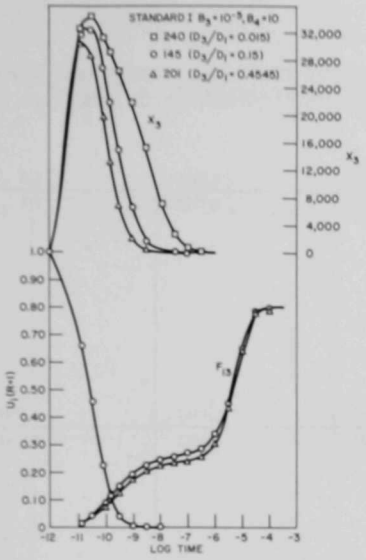
General Shapes of Solutions $U_i(R,T)$

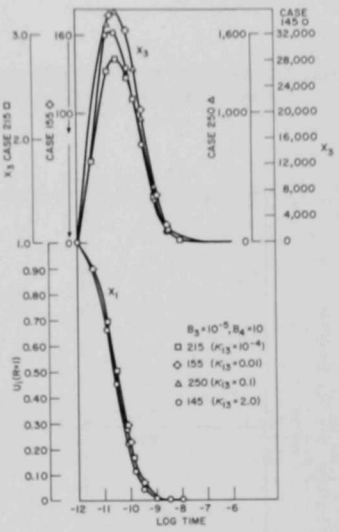


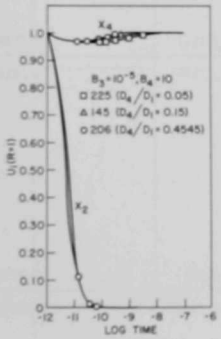
Figs. 47-51. Time Dependence of Recombination Fractions

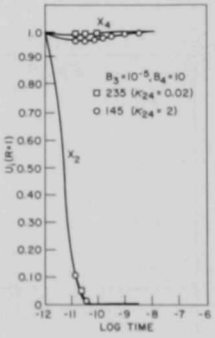


Figs. 52-57. Time Dependence of Recombination Fractions









Figs. 58-61. Time Dependence of Recombination Fractions

Table XX

CONCENTRATIONS OF REACTANTS AT VARIOUS TIMES AND POSITIONS IN SPACE FOR CASE 257: SPHERICAL GEOMETRY; STANDARD II; $B_3 = B_4 = 0$

T	P = 0	P = 9	P = 17	P = 25	P = 33
1.0	0	0.2727	0.5152	0.7576	1.0
	0	0.2727	0.5152	0.7576	1.0
0.75	0	0.1009	0.1780	0.2467	0.3084
	0	0.1033	0.2472	0.4083	0.5748
0.50	0	0.2611^{-1}	0.4527^{-1}	0.6167^{-1}	0.7569^{-1}
	0	0.2011^{-1}	0.7421^{-1}	0.1575	0.2614
0.25	0	0.2822^{-2}	0.5012^{-2}	0.6947^{-2}	0.8612^{-2}
	0	0.9436^{-3}	0.7008^{-2}	0.2258^{-1}	0.5067^{-1}
0	0	0.1233^{-9}	0.2328^{-9}	0.3422^{-9}	0.4516^{-9}
	0	0.1460^{-10}	0.1961^{-9}	0.9303^{-9}	0.2865^{-8}

Table XXI

CONCENTRATIONS OF REACTANTS AT VARIOUS TIMES AND POSITIONS IN SPACE FOR CASE 305: SPHERICAL GEOMETRY; STANDARD II; $B_3 = 10^{-5}$, $B_4 = 10$

T									
1.0	0	1.0	0.2727	1.0	0.5152	1.0	0.7576	1.0	1.0	1.0
	0	1.0	0.2727	1.0	0.5152	1.0	0.7576	1.0	1.0	1.0
0.75	0	1.0	0.1008	4491.04	0.1772	11675.78	0.2443	20495.45	0.3037	30363.72
	0	1.0	$0.5694^{(-4)}$	0.9955	$0.1466^{(-3)}$	0.9883	$0.2626^{(-3)}$	0.9795	$0.4032^{(-3)}$	0.9696
0.50	0	1.0	$0.2591^{(-1)}$	689.47	$0.4435^{(-1)}$	3528.97	$0.5920^{(-1)}$	9406.88	$0.7054^{(-1)}$	18788.33
	0	1.0		0.9993		0.9965		0.9906		0.9812
0.25	0	1.0	$0.2750^{(-2)}$	11.91	$0.4806^{(-2)}$	236.53	$0.6461^{(-2)}$	1469.55	$0.7539^{(-2)}$	5495.83
	0	1.0		1.0		0.9998		0.9985		0.9945
0	0	1.0	$0.9217^{(-14)}$	1.0	$0.1741^{(-13)}$	1.0	$0.2560^{(-13)}$	1.0	$0.3378^{(-13)}$	1.0002
	0	1.0	0	1.0	0	1.0	0	1.0	0	1.0
		0		9		17		25		33

P

Table XXII

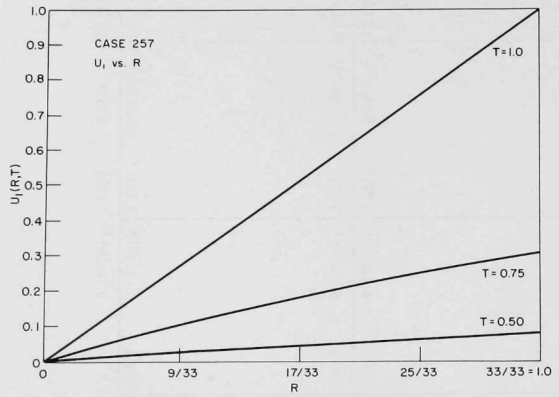
CONCENTRATIONS OF REACTANTS AT VARIOUS TIMES AND POSITIONS IN SPACE FOR CASE 303: SPHERICAL GEOMETRY; STANDARD II; $B_3 = 10^{-5}$, $B_4 = 0.1$

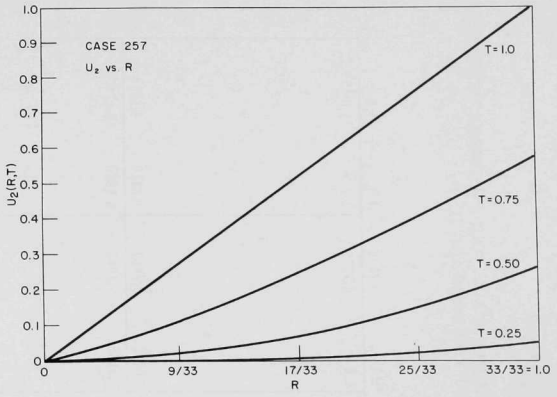
T		P = 0	9	17	25	33
1.0	0	1.0	0.2727	0.5152	0.7576	1.0
	0	1.0	0.2727	0.5152	0.7576	1.0
0.75	0	1.0	0.1009	328.34	0.1780	803.50	0.2466	1329.24	0.3082	1873.71
	0	1.0	$0.9585^{(-1)}$	0.9673	0.2300	0.9197	0.3812	0.8666	0.5383	0.8127
0.50	0	1.0	$0.2609^{(-1)}$	197.66	$0.4517^{(-1)}$	827.43	$0.6139^{(-1)}$	1867.38	$0.7512^{(-1)}$	3171.24
	0	1.0	$0.1514^{(-1)}$	0.9803	$0.5685^{(-1)}$	0.9174	0.1234	0.8134	0.2104	0.6830
0.25	0	1.0	$0.2808^{(-2)}$	18.12	$0.4963^{(-2)}$	208.60	$0.6811^{(-2)}$	920.34	$0.8283^{(-2)}$	2598.76
	0	1.0	$0.2240^{(-3)}$	0.9983	$0.1793^{(-2)}$	0.9792	$0.6432^{(-2)}$	0.9081	$0.1676^{(-1)}$	0.7402
0	0	1.0	$0.6029^{(-6)}$	0.9995	$0.1132^{(-5)}$	1.0181	$0.1654^{(-5)}$	1.2718	$0.2162^{(-5)}$	2.8250
	0	1.0	0	1.0	0	1.0	0	1.0	0	0.9998

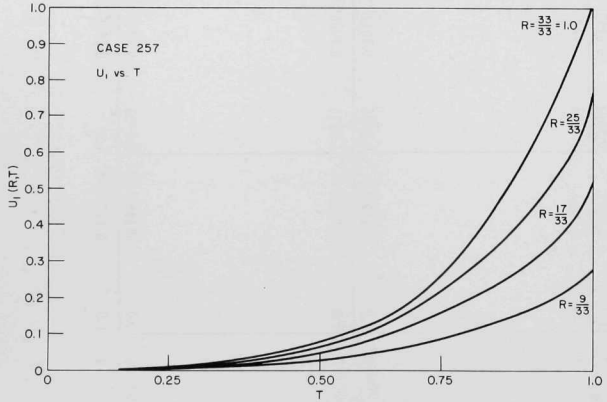
Table XXIII

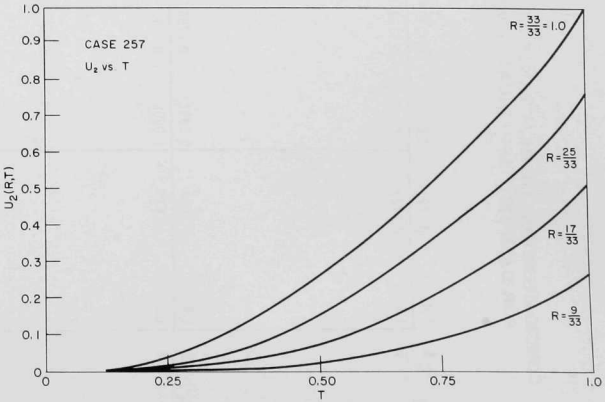
CONCENTRATIONS OF REACTANTS AT VARIOUS TIMES AND POSITIONS IN SPACE FOR CASE 301: SPHERICAL GEOMETRY; STANDARD II, $B_3 = B_4 = 10^{-5}$

T		P = 0	P = 9	P = 17	P = 25	P = 33
1.0	0	1.0	0.2727	1.0	0.5152	1.0	0.7576	1.0	1.0	1.0
	0	1.0	0.2727	1.0	0.5152	1.0	0.7576	1.0	1.0	1.0
0.75	0	1.0	0.1009	0.9992	0.1780	1.0122	0.2467	1.0320	0.3084	1.0551
	0	1.0	0.1033	1.0008	0.2472	0.9878	0.4083	0.9680	0.5747	0.9448
0.50	0	1.0	0.0261	0.9902	0.0453	1.0160	0.0617	1.0809	0.0757	1.1749
	0	1.0	0.0201	1.0098	0.797	0.9840	0.1575	0.9191	0.2614	0.8251
0.25	0	1.0	$0.2822^{(-2)}$	0.9885	$0.5012^{(-2)}$	0.9953	$0.6946^{(-2)}$	1.0656	$0.8611^{(-2)}$	1.2413
	0	1.0	$0.9000^{(-3)}$	1.0115	$0.7008^{(-2)}$	1.0047	$0.2258^{(-1)}$	0.9343	$0.5067^{(-1)}$	0.7586
0	0	1.0	$0.9857^{(-14)}$	0.9999	$0.1862^{(-13)}$	0.9999	$0.2738^{(-13)}$	0.9999	$0.3614^{(-13)}$	1.0
	0	1.0	$0.1173^{(-14)}$	1.0	$0.1576^{(-13)}$	1.0	$0.7483^{(-13)}$	0.9999	$0.2307^{(-12)}$	0.9999

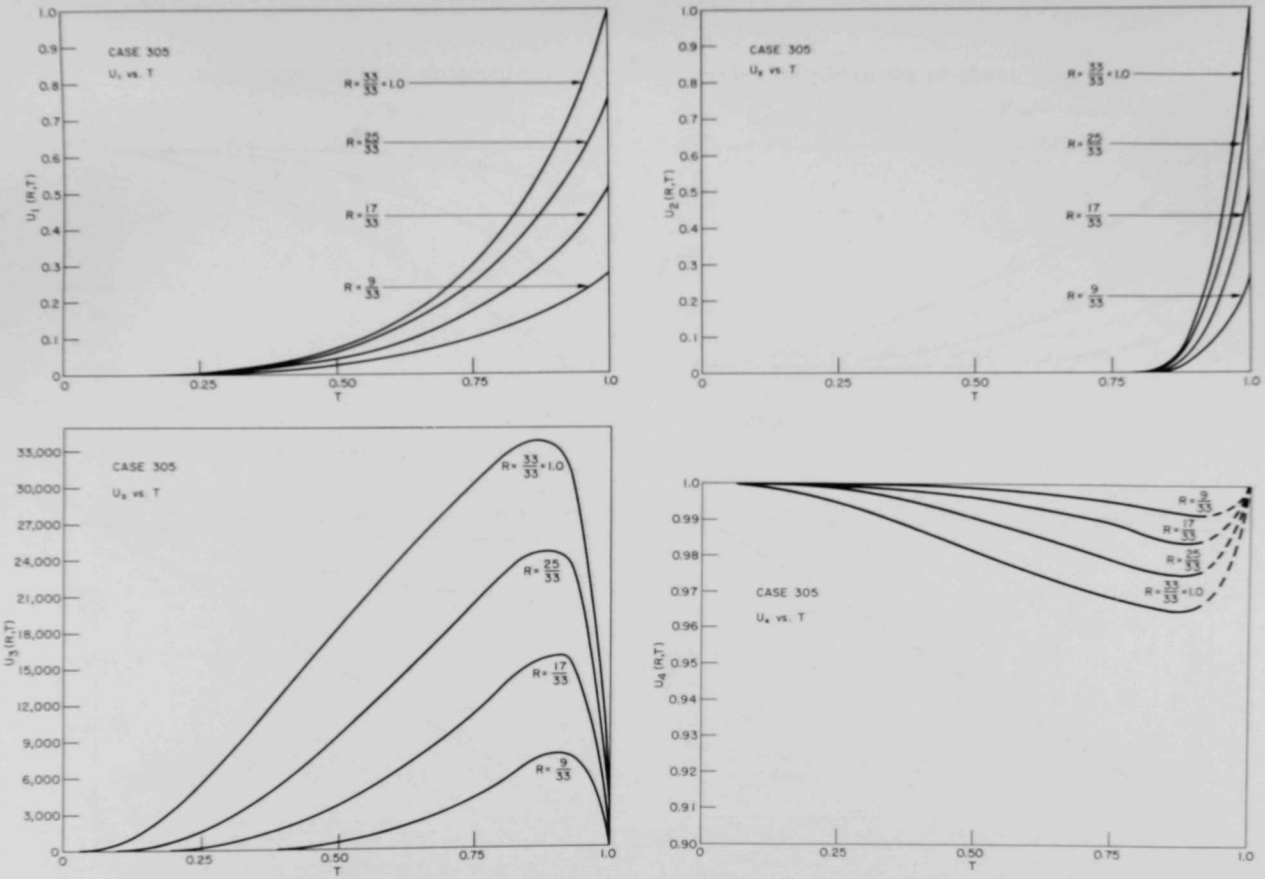




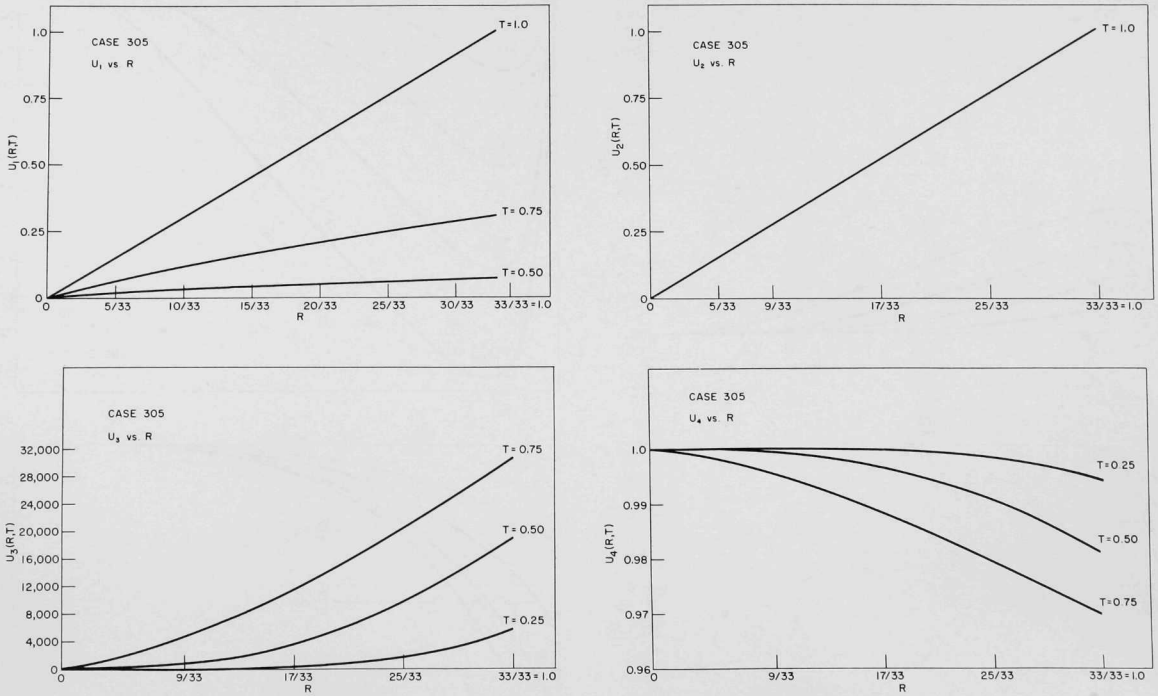




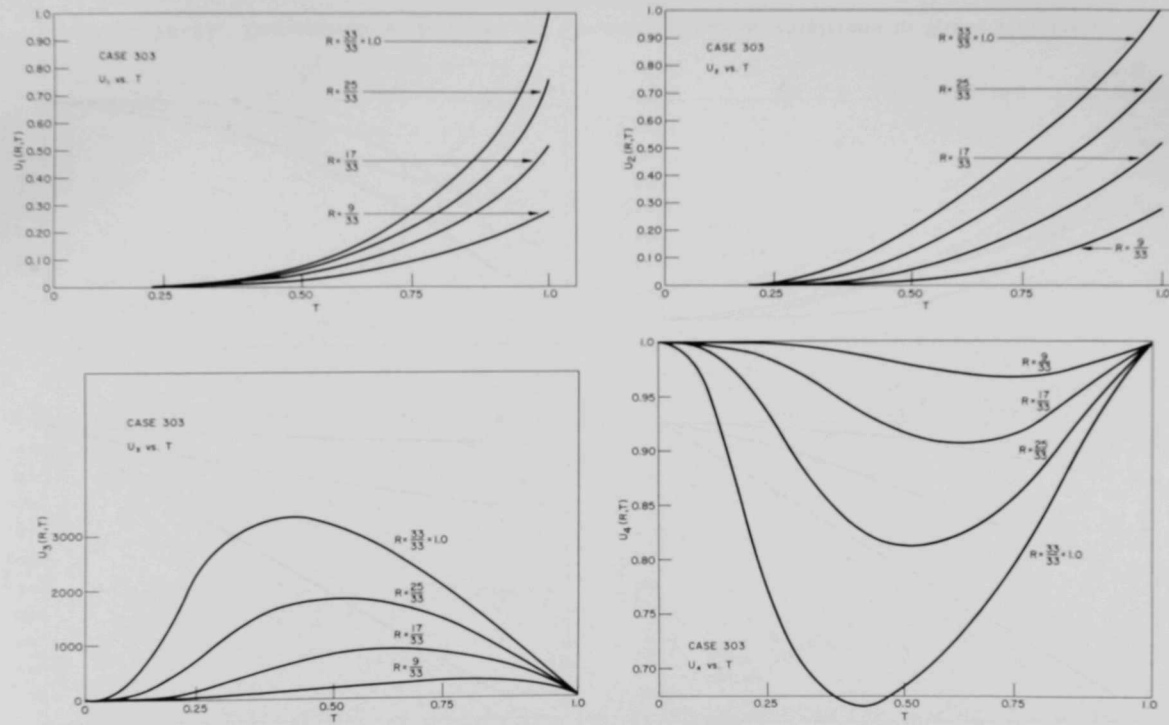
Figs. 62-65. Dependence of Normalized Concentrations on Positions in Space and Time.



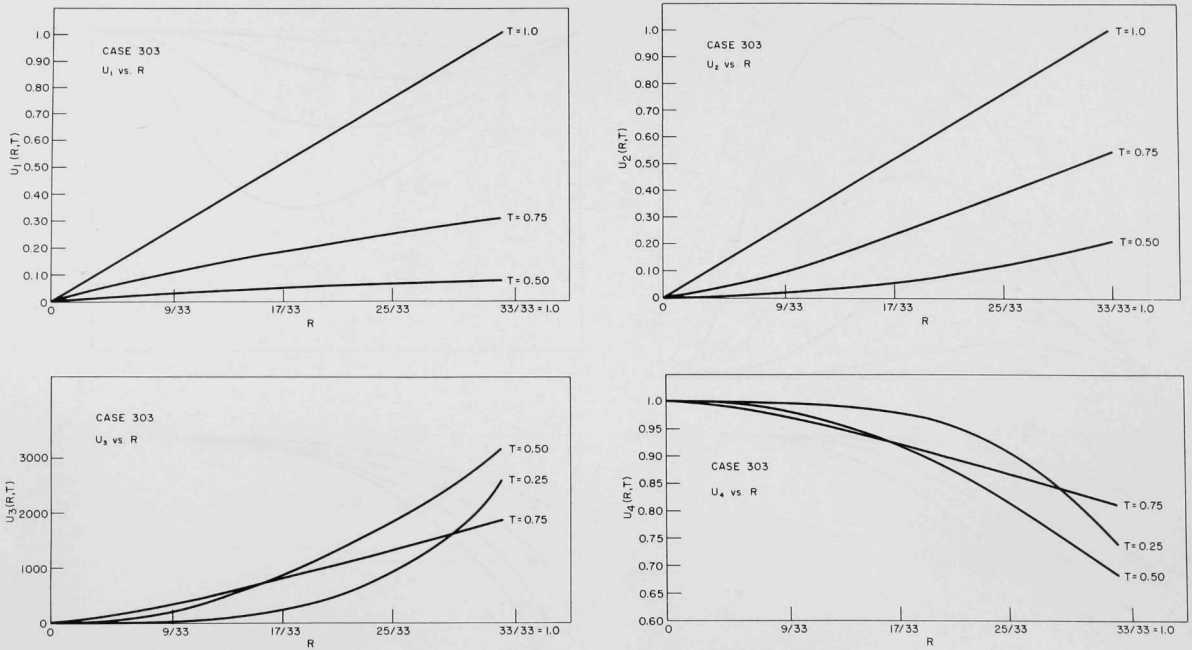
Figs. 66-69. Dependence of Normalized Concentrations on Positions in Space and Time.



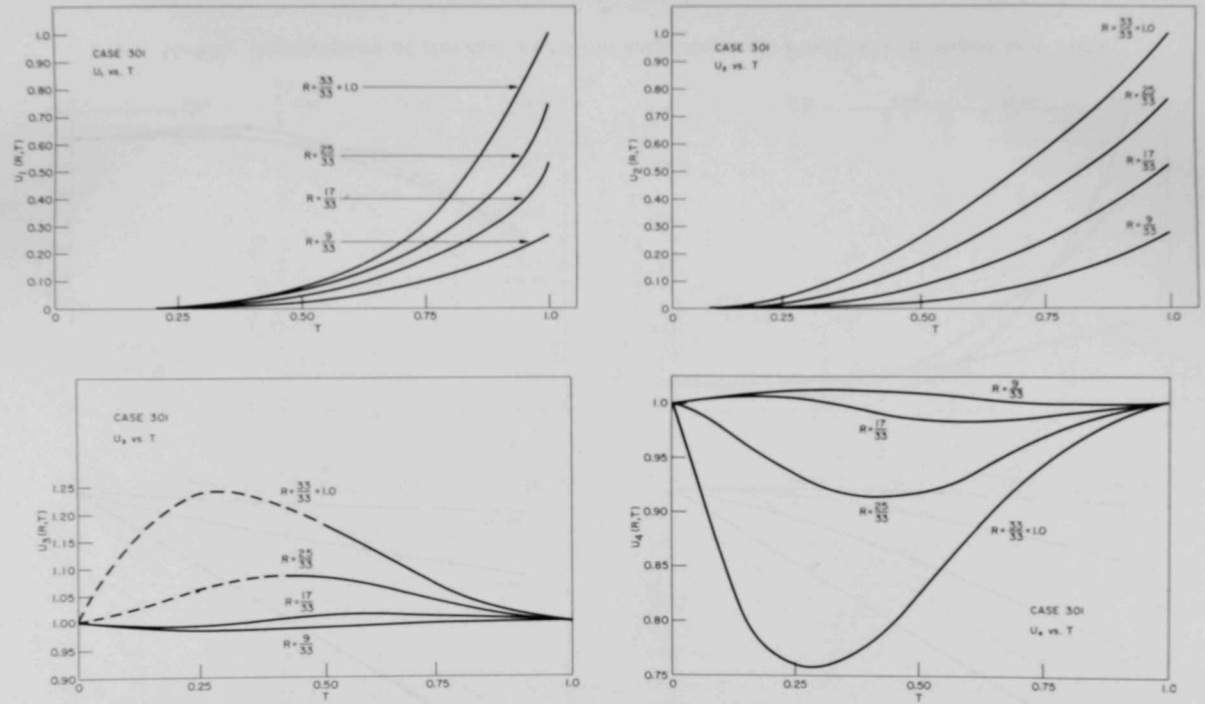
Figs. 70-73. Dependence of Normalized Concentrations on Positions in Space and Time.



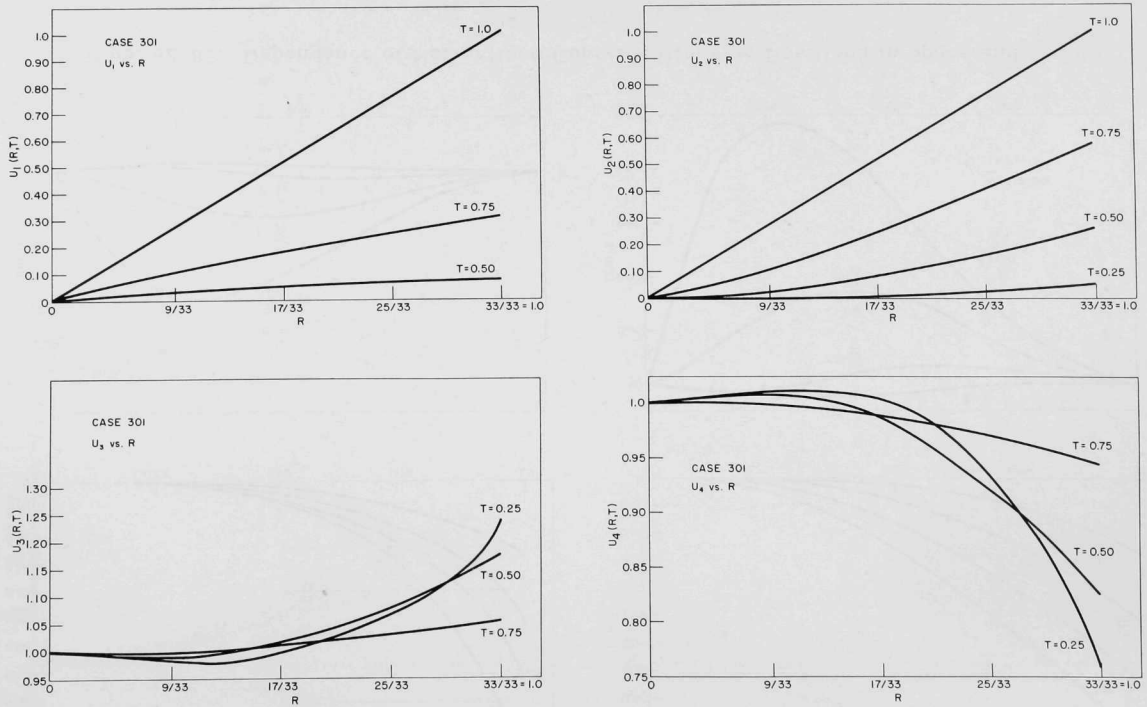
Figs. 74-77. Dependence of Normalized Concentrations on Positions in Space and Time



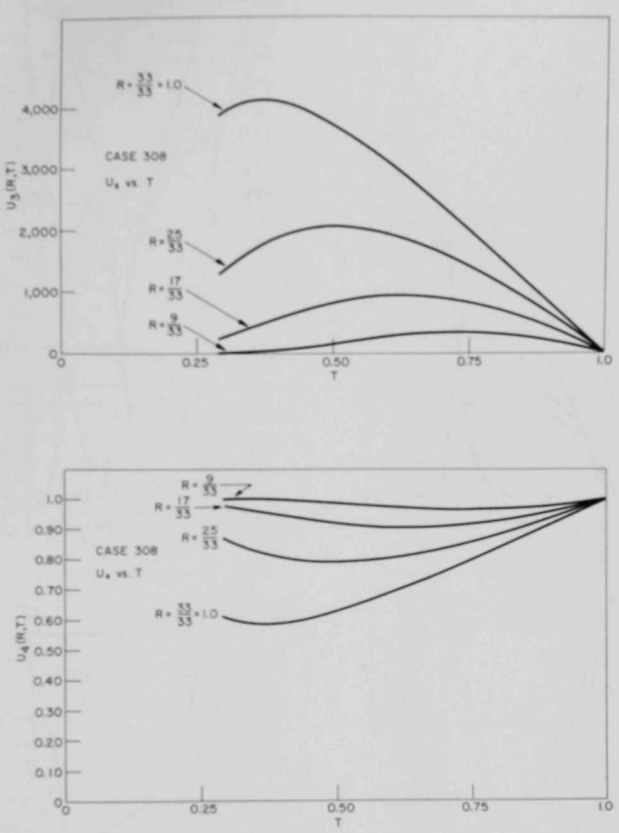
Figs. 78-81. Dependence of Normalized Concentrations on Positions in Space and Time



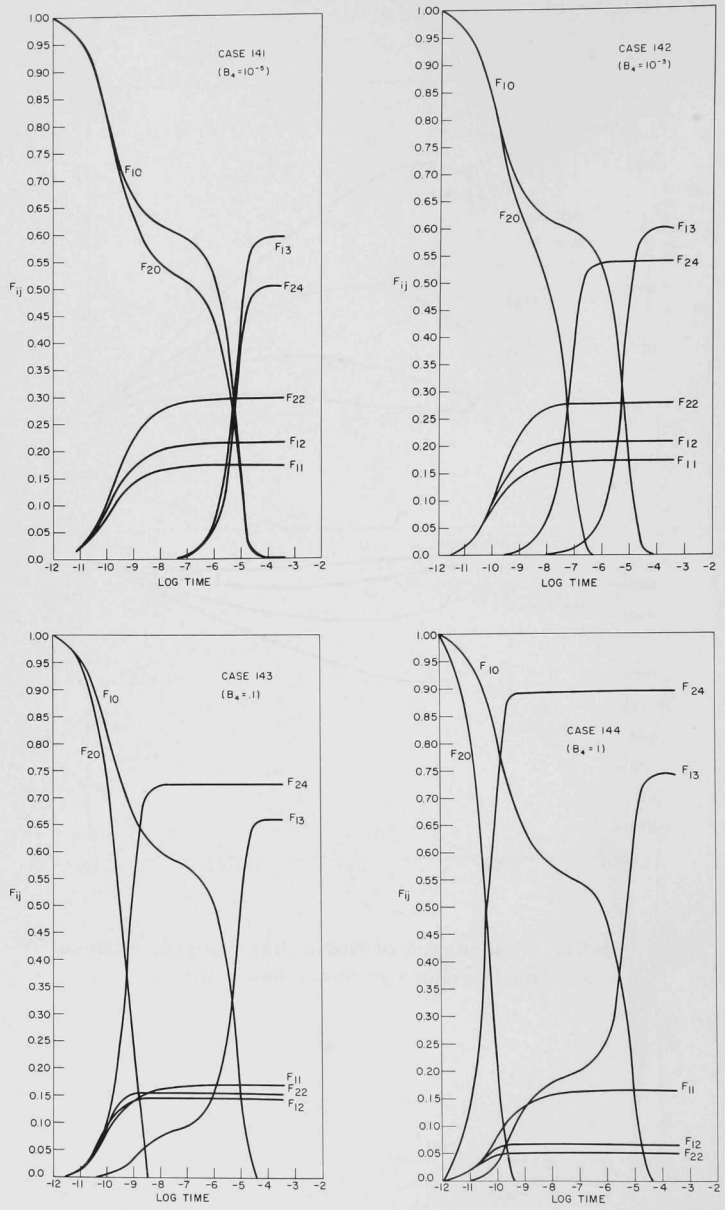
Figs. 82-85. Dependence of Normalized Concentrations on Positions in Space and Time



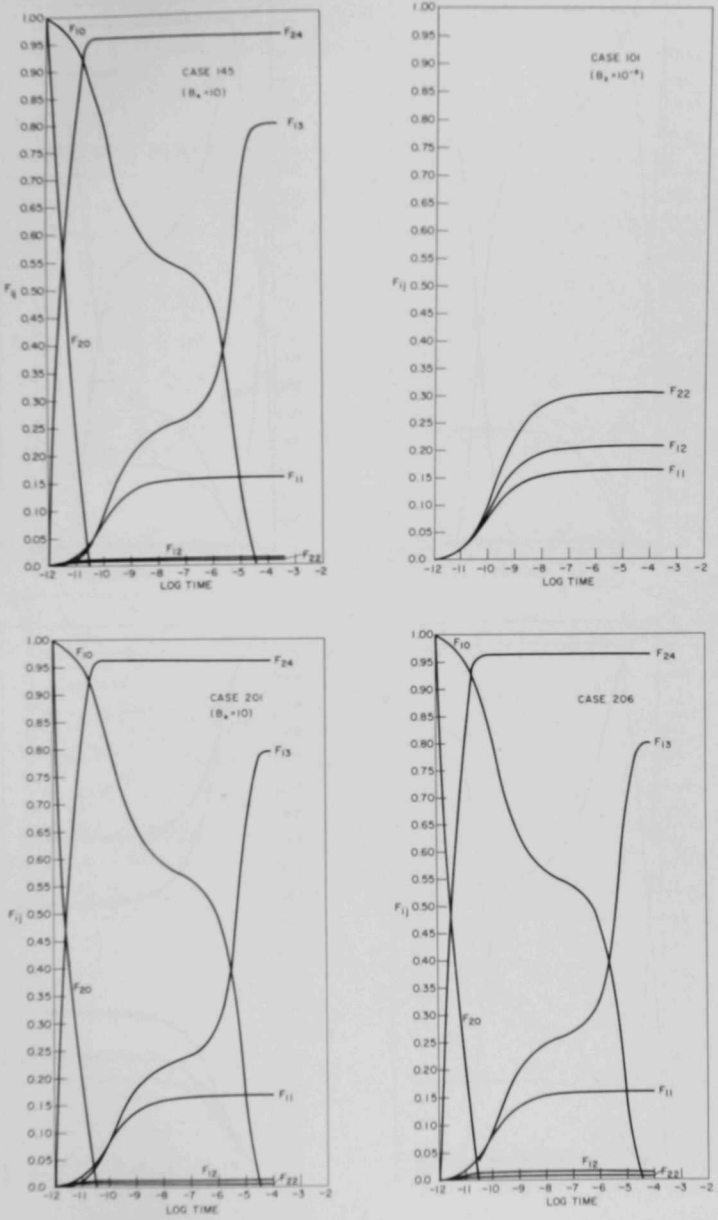
Figs. 86-89. Dependence of Normalized Concentrations on Positions in Space and Time



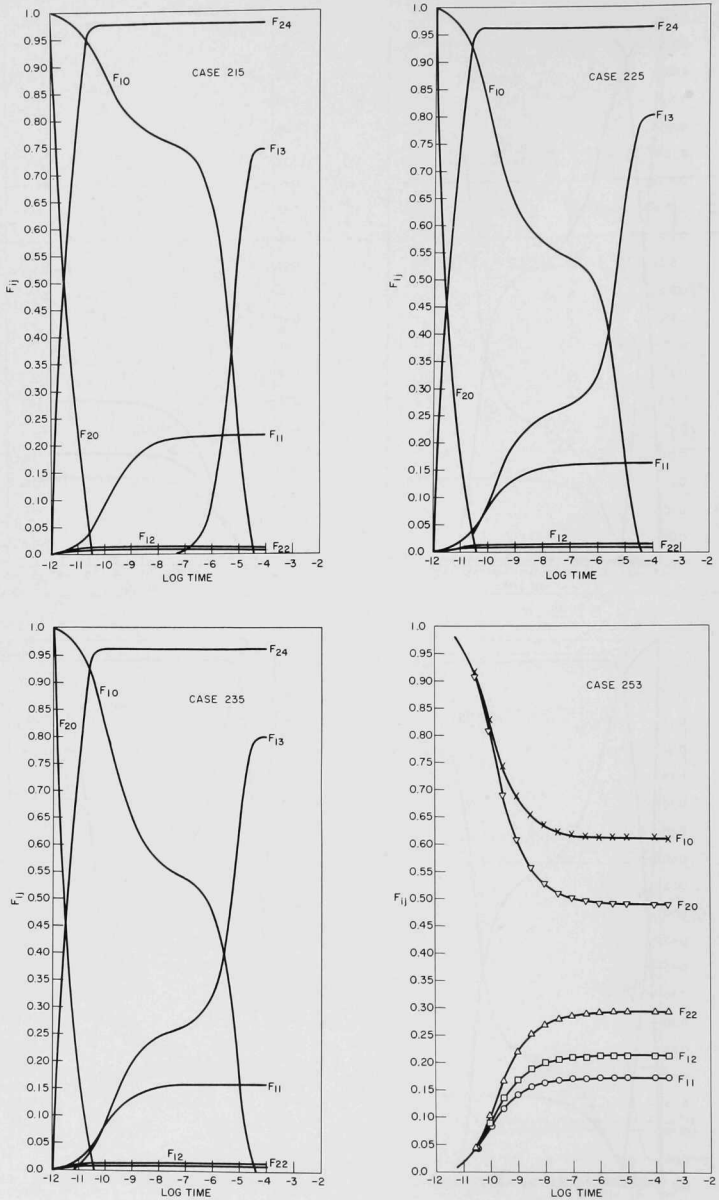
Figs. 90-91. Dependence of Normalized Concentrations on Positions in Space and Time



Figs. 92-95. Time Dependence of Recombination Fractions



Figs. 96-99. Time Dependence of Recombination Fractions



Figs. 100-103. Time Dependence of Recombination Fractions

SECTION FIVE: RESULTS OBTAINED FROM CODE C, FOR THREE PRIMARY AND ONE SECONDARY REACTION. THUS, D_3/D_1, κ_{13}, AND B_3 ARE ALL ZERO.

Table XXIV

PARAMETERS FOR STANDARD II CASES RUN WITH CODE C

Case No.	ϵ	β	E	D_2/D_1	D_4^*/D_1	κ_{12}	κ_{22}	κ_{24}^*	B_4^*
1000	2	1	0.87	0.25	0	2	0.55	0.1	0.02175
1001	2	1	0.87	0.25	1.0	2	0.55	0.1	0.02175
1002	2	1	0.87	0.25	0.5	2	0.55	0.1	0.02175
1003	2	1	0.87	0.25	0.125	2	0.55	0.1	0.02175
1004	1	1	1.60	0.25	0.125	2	0.55	0.1	0.08

Table XXV

RESULTS OF CASES DESCRIBED IN TABLE XXIV

Case No.	F_{11}	F_{12}	F_{22}	$F_{24}^* = HO_2$	$H_2 = \frac{1}{2}F_{11}$	$HO_2 = \frac{1}{2}F_{22} - F_{24}^*$
1000			No Result (unstable)			
1001	0.1670	0.2410	0.2731	0.0014	0.0835	0.1351
1002	0.1670	0.2410	0.2724	0.0023	0.0835	0.1339
1003	0.1670	0.2410	0.2720	0.0042	0.0835	0.1318
1004	0.475	0.525	0.437	0.038	0.238	0.181

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Sandra Janoucek and Joanne Griffin of Argonne National Laboratory's Applied Mathematics Division assisted with the calculations and graph plotting.

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