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SUBJECT: Reactor Studies in Two Dimensions and Two Regions

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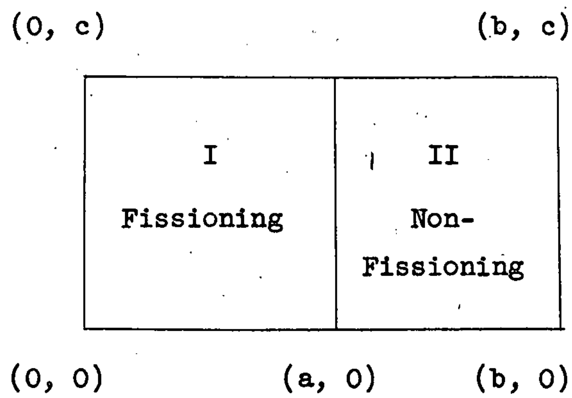
REACTOR STUDIES IN TWO DIMENSIONS AND TWO REGIONS

I. Summary

To gain insight into the reliability and rapidity of convergence of numerical methods that must in general be used for reactor calculations in two dimensions, a rather simple model is chosen and extensively explored. The model is indicated by the following figure, differential equations and boundary conditions.



(I.1) $$\varphi_{xx} + \varphi_{yy} + B^2 \varphi = 0 \qquad \begin{cases} 0 < x < a \\ 0 < y < c \end{cases}$$

(I.2) $$\varphi_{xx} + \varphi_{yy} - K^2 \varphi = 0 \qquad \begin{cases} a < x < b \\ 0 < y < c \end{cases}$$

(I.3) Boundary Conditions: (a) $\varphi(0, y) = \varphi(b, y) = \varphi(x, 0) = \varphi(x, c) = 0$

(b) $D_1 \varphi_1'(a) = D_2 \varphi_2'(a)$

(c) $\varphi_1(a) = \varphi_2(a)$.

The quantities D_1 , D_2 and K^2 are assumed known. The values B^2 form the eigenvalues of the system and one is interested in finding the fundamental eigenvalue.

This system lends itself to analytic solution, and the results obtained here form the basis for comparison with the results of various numerical procedures. The solution can be written in the form,

$$\text{(I.4)} \qquad \tan ax + Lx = 0$$

with

$$\text{(I.5)} \qquad x = \sqrt{B^2 - \frac{\pi^2}{b^2}} \qquad \text{and} \qquad L = \frac{D_1 \tanh \sqrt{K^2 + \frac{\pi^2}{b^2}}\,(1 - a)}{D_2 \sqrt{K^2 + \frac{\pi^2}{b^2}}} .$$

For simplicity it has been assumed that $b = c = 1$.

II. The Difference Approximation

For numerical solution one would wish to replace the differential system (I.1 - I.3) with a finite difference scheme. As a first approach the following are used:

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(II.1)
$$\varphi_x \approx \frac{\varphi_{x+h,y} - \varphi_{x-h,y}}{2h}$$

(II.2)
$$\varphi_{xx} \approx \frac{\varphi_{x+h,y} - 2\varphi_{x,y} + \varphi_{x-h,y}}{h^2} \quad .$$

These are second-order approximations to the first and second derivatives. By this it is meant that the error terms will involve h^2 . In this note this will be called a crude approximation to the interior points and a crude approximation to the normal derivative at the interface (crude-crude). The difference system resulting from the use of these approximations is as follows:

(II.3)
$$\frac{1}{h^2}(\varphi_{i+1,j} - 2\varphi_{i,j} + \varphi_{i-1,j}) + \frac{1}{h^2}(\varphi_{i,j+1} - 2\varphi_{i,j} + \varphi_{i,j-1}) + + B^2 \varphi_{i,j} = 0$$

(II.4)
$$\frac{1}{h^2}(\varphi_{i+1,j} - 2\varphi_{i,j} + \varphi_{i-1,j}) + \frac{1}{h^2}(\varphi_{i,j+1} - 2\varphi_{i,j} + \varphi_{i,j-1}) - - K^2 \varphi_{i,j} = 0 \quad .$$

With the boundary conditions as given in (I.3), analytic solution of this difference system is possible and the result can be written in the form,

(II.5)
$$\tan ax + L \sin(hx) = 0$$

3 7 6 4

with

(II.6) $$L = \frac{D_1 \tanh (1 - a)\gamma}{D_2 \sinh (h\gamma)}$$

$$\gamma = \frac{1}{h} \cosh^{-1} \left[2 + \frac{(hK)^2}{2} - \cos \pi h \right]$$

$$B^2 = \frac{2}{h^2} \left[2 - \cos(hx) - \cos \pi h \right] .$$

In using a difference scheme one has two choices to improve the accuracy. First, the size of h can be taken smaller, that is more mesh points could be used, or one can seek further improvement by finding a better difference approximation to the differential system. A difference scheme with fourth order accuracy can be written as follows,

(II.7) $$\left(4 + \frac{B^2 h^2}{2}\right) (\varphi_{i+1,j} + \varphi_{i-1,j} + \varphi_{i,j+1} + \varphi_{i,j-1}) + (4 B^2 h^2 - 20)\varphi_{i,j} + $$
$$+ (\varphi_{i+1,j+1} + \varphi_{i-1,j+1} + \varphi_{i+1,j-1} + \varphi_{i-1,j-1}) = 0$$

(II.8) $$\left(4 - \frac{K^2 h^2}{2}\right) (\varphi_{i+1,j} + \varphi_{i-1,j} + \varphi_{i,j+1} + \varphi_{i,j-1}) + (-4 K^2 h^2 - 20)\varphi_{i,j} + $$
$$+ (\varphi_{i+1,j+1} + \varphi_{i-1,j+1} + \varphi_{i+1,j-1} + \varphi_{i-1,j-1}) = 0$$

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and a fourth order approximation to the normal derivative at the interface,

$$\varphi_x \approx \left(\frac{1}{3h} + \frac{B^2 h}{12}\right) (\varphi_{i+1,j} - \varphi_{i-1,j}) + \frac{1}{12h} (\varphi_{i+1,j+1} + \varphi_{i+1,j-1} - \varphi_{i-1,j+1} - \varphi_{i-1,j-1}) . \tag{II.9}$$

This approximation will be referred to as the refined-refined case. Analytic solution is again possible and the result takes the form,

$$\tan ax + L \sin(hx) \left[\frac{A_1 + B^2 h^2}{A_1 - K^2 h^2}\right] = 0 \tag{II.10}$$

with

$$A_1 = 4 + 2 \cos \pi h^2 \tag{II.11}$$

$$L = \frac{D_1 \tanh \gamma(1 - a)}{D_2 \sinh (\gamma h)}$$

$$\gamma = \frac{1}{h} \cosh^{-1} \left[\frac{20 + 4K^2 h^2 + (\frac{K^2 h^2}{2} - 4)(2 \cos \pi h)}{8 - K^2 h^2 + 4 \cos \pi h}\right]$$

$$B^2 = \frac{20 - 4 \cos(hx) \cos \pi h - 8 \cos(hx) - 8 \cos \pi h}{h^2 \left[\cos(hx) + \cos \pi h + 4\right]} .$$

Since, for numerical solution, the use of the refined approximation for the derivative greatly complicates the problem, it was thought advisable to investigate the possibility of using a refined approximation for the interior points and a crude approximation for the derivative (refined-crude). In a numerical procedure this would be almost as easy to apply as the crude-crude approximation. However, as can be seen from the numerical results in the table at the end of this note, nothing is to be gained by this approach. Analytic solution of the refined-crude approximation gives as a result,

$$\tan ax + L \sin(hx) = 0 \tag{II.12}$$

with

$$L = \frac{D_1 \tanh (1 - a)\gamma}{D_2 \sinh(\gamma h)} \tag{II.13}$$

$$\gamma = \frac{1}{h} \cosh^{-1} \left[\frac{20 + 4 K^2 h^2 + (K^2 h^2 - 8)\cos \pi h}{8 - K^2 h^2 + 4 \cos \pi h} \right]$$

$$K^2 = \frac{20 - 4 \cos \pi h \cos(xh) - 8 \cos \pi h - 8 \cos(xh)}{h^2 \left[\cos(xh) + \cos \pi h + 4\right]}$$

A series of calculations were made for each of the four cases referred to above. It was seen that all variations could be observed by varying only one of the parameters D_1 , D_2 , K^2 and a . With this in mind D_1 , K^2 and a

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were held constant and only D_2 and the mesh size (h) were varied.

III. Numerical Solution of the Difference System

In general, of course, analytic solution of the differential or approximating difference system is not possible so one must turn to a numerical procedure for the solution of the difference system. One such method was coded for the Oracle so that reliability and computing time could be evaluated. A crude difference approximation was used. The following difference equations are to hold in the various regions:

$$\varphi_{i+1,j} + \varphi_{i-1,j} + \varphi_{i,j-1} + \varphi_{i,j+1} - 4\varphi_{i,j} + B^2 h^2 \varphi_{i,j} = 0 \tag{III.1}$$

for points in the fissionable region except on boundaries and

$$\varphi_{i+1,j} + \varphi_{i-1,j} + \varphi_{i,j+1} + \varphi_{i,j-1} - (4 + K^2 h^2)\varphi_{i,j} = 0 \tag{III.2}$$

for points in the non-fissionable region except on boundaries, and

$$\frac{2D_2}{D_1 + D_2}\varphi_{i+1,j} + \frac{2D_1}{D_1 + D_2}\varphi_{i-1,j} + \varphi_{i,j+1} + \varphi_{i,j-1} - \left(4 + \frac{D_2 K^2 h^2}{D_1+D_2}\right)\varphi_{i,j} + \frac{D_1 B^2 h^2}{D_1 + D_2}\varphi_{i,j} = 0 \tag{III.3}$$

for points on the interface.

For solution the fundamental eigenvalue (B^2) of the following system is required.

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(III.4) $$A \bar{\Phi} + B^2 M \bar{\Phi} = 0$$

where,

A is a square matrix whose order is the number of mesh points to be used.

M is a singular diagonal matrix of the same order as A .

The matrix A is not symmetric, the assymmetry being due to the equation which holds for points along the interface.

An iterative scheme with the steps as indicated in the following was used:

(a) A vector $\bar{\Phi}^{(0)}$ is assumed.

(b) The vector $D^{(0)} = B^2 M \bar{\Phi}$ is computed where a first estimation of B_0^2 is made.

(c) The system $A \bar{\Phi}^{(1)} + D_0 = 0$ is solved.

(d) The vector $D^{(1)*} = M \bar{\Phi}^{(1)}$ is computed.

(e) The quantity

$$B_1^2 \approx \frac{\Sigma D^{(0)}}{\Sigma D^{(1)*}}$$

is found.

(f) A new $D^{(1)} = B_1^2 D^{(1)*}$ is found and the cycle is reentered at (c) until convergence to B^2 is complete.

Solution of the system $A \bar{\Phi} + D = 0$ is the major problem as far as computing time is concerned. The method used to solve this system is that of

Richardson as given by Young.[1] It was found that this method was satisfactory in that the B^2 from the analytic solution could be duplicated to as many as 8 or 9 digits in some 15 minutes of computing time. The computing time was appreciably shortened by a proper choice and rearrangement of the relaxation factors which are used to accelerate convergence in Richardson's method. The overall convergence time can be improved by a proper adjustment of the convergence criteria (ϵ) in the system $A \Phi + D = 0$. The best approach seems to be to begin with a very lax ϵ, since one usually starts with a flat source or at least a rather poor one, and to make this progressively more strict as subsequent passes are made through the major computing loop. As an example it was found that the system $A \Phi + D = 0$ had to be iterated on some 500 times for overall convergence if a small ϵ was maintained from the beginning throughout to convergence, while only 300 iterations were necessary for a progressively decreasing ϵ. Throughout all of these investigations approximately 300 mesh points were used.

IV. Conclusions

A survey of results is given in the tables and in the graphs. The tables speak for themselves as regard to the accuracy of the different methods involved. It should be noted that the refined-crude scheme is no better and sometimes worse than the crude-crude approximation. Also, one should note that while the results of the crude approximation always are somewhat below those of the true solution the results of the refined case show values slightly above the true result. This phenomena has been justified by analytic considerations.

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[1] Young, David, "On Richardson's Method for Solving Linear Systems with Positive Definite Matrices", Journal of Mathematics and Physics, 32(1953-4) pp. 243-255.

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The results would indicate that one would be justified in complicating the computational set-up by using the refined approximation in order to gain the advantage of the increased accuracy with much fewer mesh points.

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D_1	D_2	Exact B^2	1/h	Crude-B^2	Crude $\triangle B^2$	Refined-B^2	Crude $\triangle B^2$	Refined-B^2	Refined $\triangle B^2$
1	1/5	22.3852	5	21.8630	-.5222	22.8163	+.4311	22.4214	+.0362
			10	22.2541	.1311	22.4839	.0987	22.3876	.0024
			15	22.3269	.0583	22.4284	.0432	22.3857	.0005
			18	22.3447	.0405	22.4150	.0298	22.3854	.0002
			20	22.3524	.0328	22.4093	.0241	22.3853	.0001
			25	22.3642	.0210	22.4006	.0154	22.3852	.0000
			30	22.3706	.0146	22.3959	.0107	22.3852	.0000
			35	22.3745	.0107	22.3930	.0078	22.3852	.0000
			40	22.3770	.0082	22.3912	.0060	22.3852	.0000
			45	22.3787	.0065	22.3899	.0047	22.3852	.0000
1	1/5	22.3852	50	22.3799	-.0053	22.3890	+.0038	22.3852	.0000
1	1/4	22.9898	5	22.4934	-.4964	23.5230	+.5532	23.0336	+.0438
			10	22.8654	.1244	23.1120	.1222	22.9928	.0030
			15	22.9345	.0553	23.0433	.0535	22.9904	.0006
			18	22.9514	.0384	23.0268	.0370	22.9901	.0003
			20	22.9587	.0311	23.0197	.0299	22.9900	.0002
			25	22.9699	.0199	23.0089	.0191	22.9899	.0001
			30	22.9760	.0138	23.0031	.0133	22.9899	.0001
			35	22.9797	.0101	22.9995	.0097	22.9898	.0000
			40	22.9820	.0078	22.9973	.0075	22.9898	.0000
			45	22.9837	.0061	22.9957	.0059	22.9898	.0000
1	1/4	22.9898	50	22.9848	-.0050	22.9946	+.0048	22.9898	.0000
1	1/3	23.9513	5	23.4932	-.4581	24.6486	+.6973	24.0080	+.0567
			10	23.8368	.1145	24.1111	.1598	23.9551	.0038
			15	23.9005	.0508	24.0212	.0699	23.9521	.0008
			18	23.9160	.0353	23.9997	.0484	23.9517	.0004
			20	23.9227	.0286	23.9904	.0391	23.9516	.0003
			25	23.9330	.0183	23.9763	.0250	23.9514	.0001
			30	23.9386	.0145	23.9686	.0173	23.9514	.0001
			35	23.9420	.0093	23.9640	.0127	23.9514	.0001
			40	23.9442	.0071	23.9611	.0098	23.9513	.0000
			45	23.9457	.0056	23.9590	.0077	23.9513	.0000
1	1/3	23.9513	50	23.9468	-.0045	23.9576	+.0063	23.9513	.0000
1	1/2	25.7143	5	25.3120	-.4023	26.7120	+.9977	25.7966	+.0823
			10	25.6146	.0997	25.9429	.2286	25.7199	.0056
			15	25.6701	.0442	25.8143	.1000	25.7155	.0012
			18	25.6836	.0307	25.7835	.0692	25.7149	.0006
			20	25.6895	.0248	25.7703	.0560	25.7147	.0004
			25	25.6984	.0159	25.7500	.0357	25.7145	.0002
			30	25.7033	.0110	25.7391	.0248	25.7144	.0001
			35	25.7062	.0080	25.7325	.0182	25.7144	.0001
			40	25.7081	.0062	25.7282	.0139	25.7143	.0000
			45	25.7094	.0049	25.7253	.0110	25.7143	.0000
1	1/2	25.7143	50	25.7104	-.0039	25.7232	+.0089	25.7143	.0000

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D_1	D_2	Exact B^2	1/h	Crude- B^2	Crude $\triangle B^2$	Refined- B^2	Crude $\triangle B^2$	Refined- B^2	Refined $\triangle B^2$
1	1	29.9536	5	29.5489	-.4047	31.5927	+1.6391	30.1023	+.1487
			10	29.8591	.0945	30.3329	.3793	29.9637	.0101
			15	29.9121	.0415	30.1198	.1662	29.9556	.0020
			18	29.9249	.0486	30.0686	.1150	29.9546	.0010
			20	29.9304	.0232	30.0466	.0930	29.9542	.0006
			25	29.9387	.0149	30.0130	.0594	29.9538	.0002
			30	29.9433	.0103	29.9948	.0412	29.9537	.0001
			35	29.9460	.0076	29.9838	.0302	29.9536	.0000
			40	29.9478	.0058	29.9767	.0231	29.9536	.0000
			45	29.9490	.0046	29.9719	.0183	29.9536	.0000
1	1	29.9536	50	29.9499	-.0037	29.9684	+.0148	29.9536	.0000
1	2	35.3444	5	34.4707	-.8737	37.3843	+2.0399	35.5555	+.2111
			10	35.1508	.1936	35.8377	.4933	35.3591	.0147
			15	35.2604	.0840	35.5620	.2176	35.3474	.0030
			18	35.2864	.0580	35.4952	.1508	35.3459	.0015
			20	35.2975	.0469	35.4665	.1221	35.3454	.0010
			25	35.3145	.0299	35.4224	.0780	35.3448	.0004
			30	35.3237	.0207	35.3986	.0542	35.3446	.0002
			35	35.3292	.0152	35.3842	.0398	35.3445	.0001
			40	35.3328	.0116	35.3749	.0305	35.3445	.0001
			45	35.3352	.0092	35.3685	.0241	35.3444	.0000
1	2	35.3444	50	35.3370	-.0074	35.3639	+.0195	35.3444	.0000
1	3	38.5124	5	37.0446	-1.4678	40.4645	+1.9521	38.7232	+.2108
			10	38.1811	.3313	39.0053	.4929	38.5274	.0150
			15	38.3681	.1443	38.7313	.2189	38.5155	.0031
			18	38.4127	.0997	38.6644	.1520	38.5139	.0015
			20	38.4318	.0806	38.6355	.1231	38.5134	.0010
			25	38.4610	.0514	38.5912	.0788	38.5128	.0004
			30	38.4768	.0356	38.5671	.0547	38.5126	.0002
			35	38.4863	.0261	38.5526	.0402	38.5125	.0001
			40	38.4924	.0200	38.5432	.0308	38.5125	.0001
			45	38.4966	.0158	38.5367	.0243	38.5124	.0000
1	3	38.5124	50	38.4996	-.0128	38.5321	+.0197	38.5124	.0000
1	4	40.5540	5	38.5709	-1.9831	42.3089	+1.7549	40.7405	+.1865
			10	40.0963	.4577	41.0132	.4592	40.5677	.0137
			15	40.3538	.2002	40.7591	.2051	40.5568	.0028
			18	40.4155	.1385	40.6966	.1426	40.5553	.0013
			20	40.4420	.1120	40.6695	.1155	40.5549	.0009
			25	40.4825	.0715	40.6280	.0740	40.5543	.0003
			30	40.5044	.0496	40.6054	.0514	40.5542	.0002
			35	40.5176	.0364	40.5918	.0378	40.5541	.0001
			40	40.5261	.0279	40.5829	.0289	40.5541	.0001
			45	40.5320	.0220	40.5768	.0228	40.5540	.0000
1	4	40.5540	50	40.5362	-.0178	40.5725	+.0185	40.5540	.0000

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D_1	D_2	Exact B^2	1/h	Crude-B^2	Crude $\triangle B^2$	Refined-B^2	Crude $\triangle B^2$	Refined-B^2	Refined $\triangle B^2$
1	5	41.9654	5	39.5672	-2.3982	43.5205	+1.5551	42.1216	+.1562
			10	41.4021	.5633	42.3848	.4194	41.9773	.0119
			15	41.7182	.2472	42.1536	.1882	41.9678	.0024
			18	41.7943	.1711	42.0964	.1310	41.9666	.0012
			20	41.8270	.1384	42.0716	.1062	41.9662	.0008
			25	41.8770	.0884	42.0335	.0681	41.9657	.0003
			30	41.9041	.0613	42.0127	.0473	41.9655	.0001
			35	41.9204	.0450	42.0002	.0348	41.9655	.0001
			40	41.9309	.0345	41.9920	.0266	41.9654	.0000
			45	41.9382	.0272	41.9864	.0210	41.9654	.0000
1	5	41.9654	50	41.9434	-.0220	41.9824	+.0170	41.9654	.0000
1	8	44.3878	5	41.7180	-2.6698	45.4856	+1.0978	44.4618	+.0740
			10	43.6074	.7804	44.7062	.3184	44.3945	.0067
			15	44.0432	.3446	44.5323	.1445	44.3892	.0014
			18	44.1489	.2389	44.4886	.1008	44.3884	.0006
			20	44.1944	.1934	44.4696	.0818	44.3882	.0004
			25	44.2641	.1237	44.4403	.0525	44.3879	.0001
			30	44.3020	.0858	44.4243	.0365	44.3878	.0000
			35	44.3247	.0631	44.4146	.0268	44.3878	.0000
			40	44.3395	.0483	44.4084	.0170	44.3878	.0000
			45	44.3497	.0381	44.4040	.0162	44.3878	.0000
1	8	44.3878	50	44.3569	-.0309	44.4009	+.0131	44.3878	.0000

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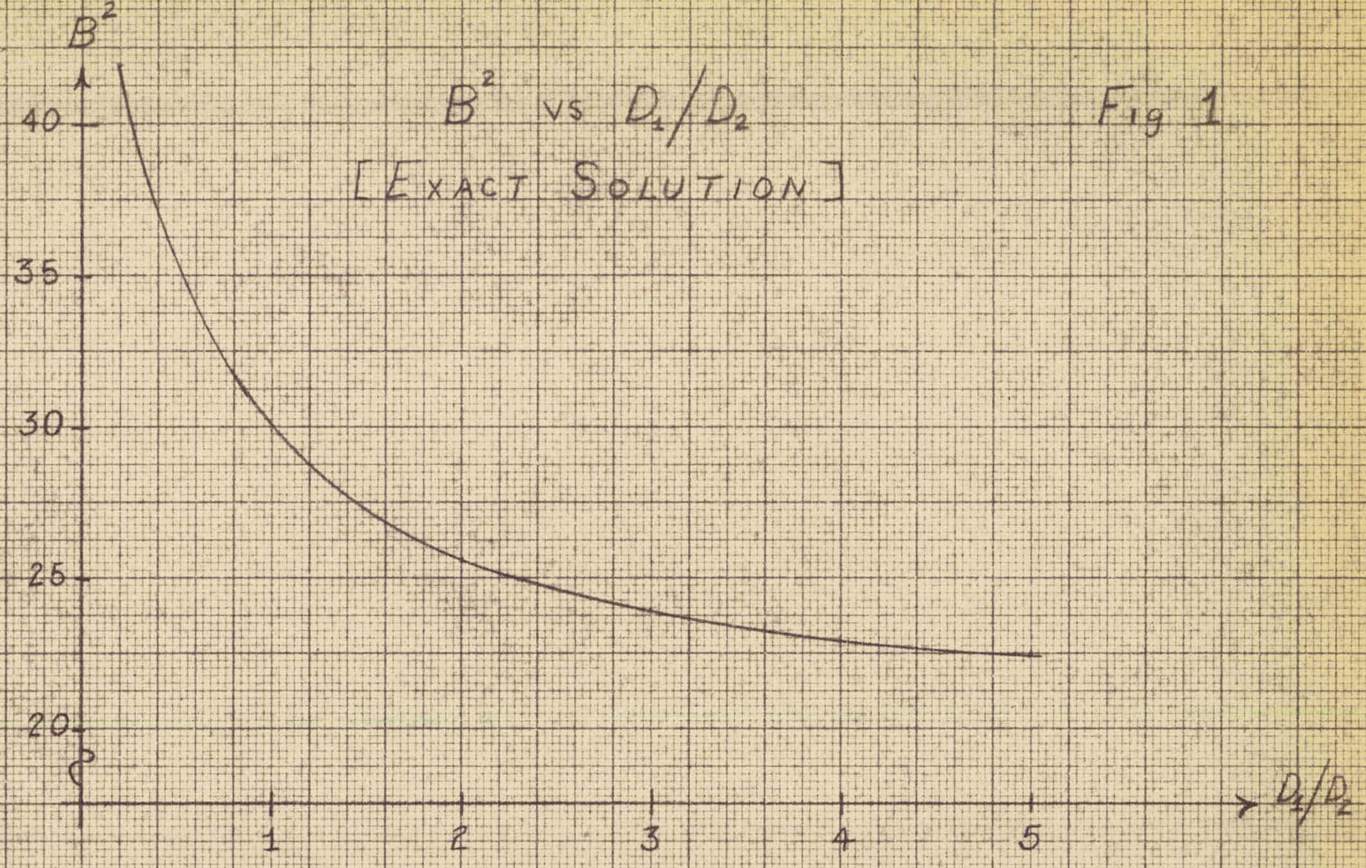

B^2 vs D_1/D_2
[Exact Solution]
B^2
40
35
30
25
20
1
2
3
4
5
D_1/D_2

Fig 1

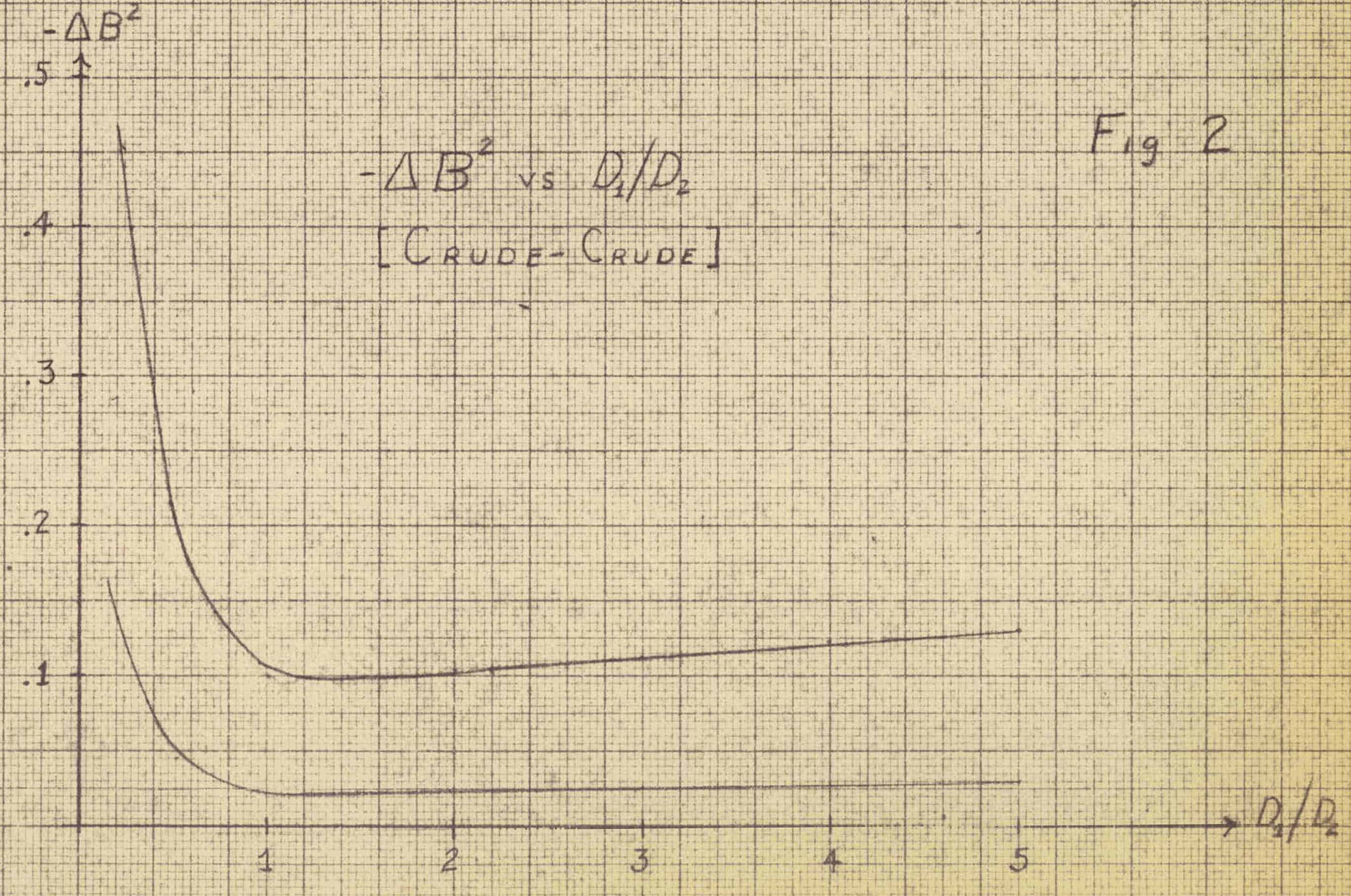
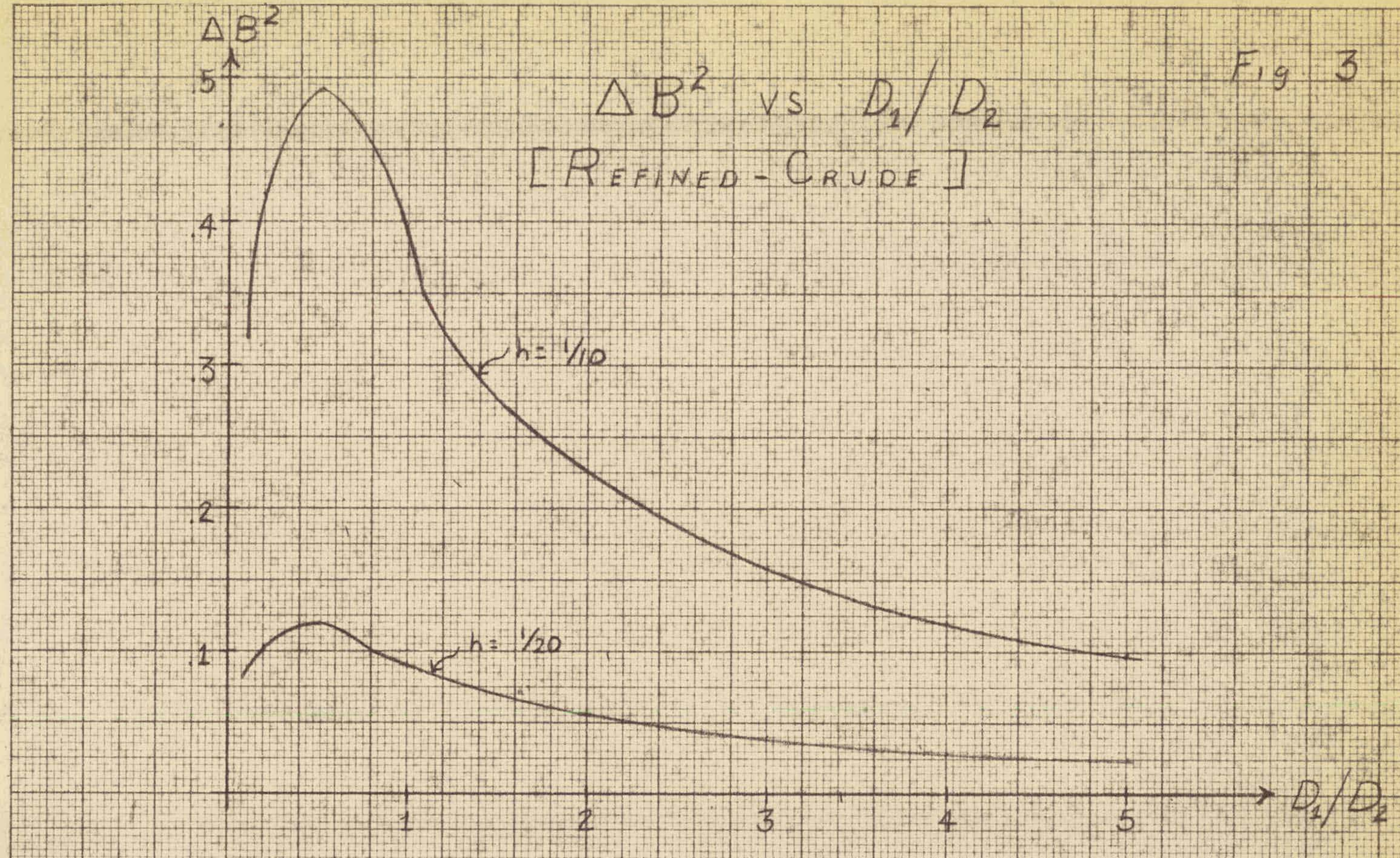
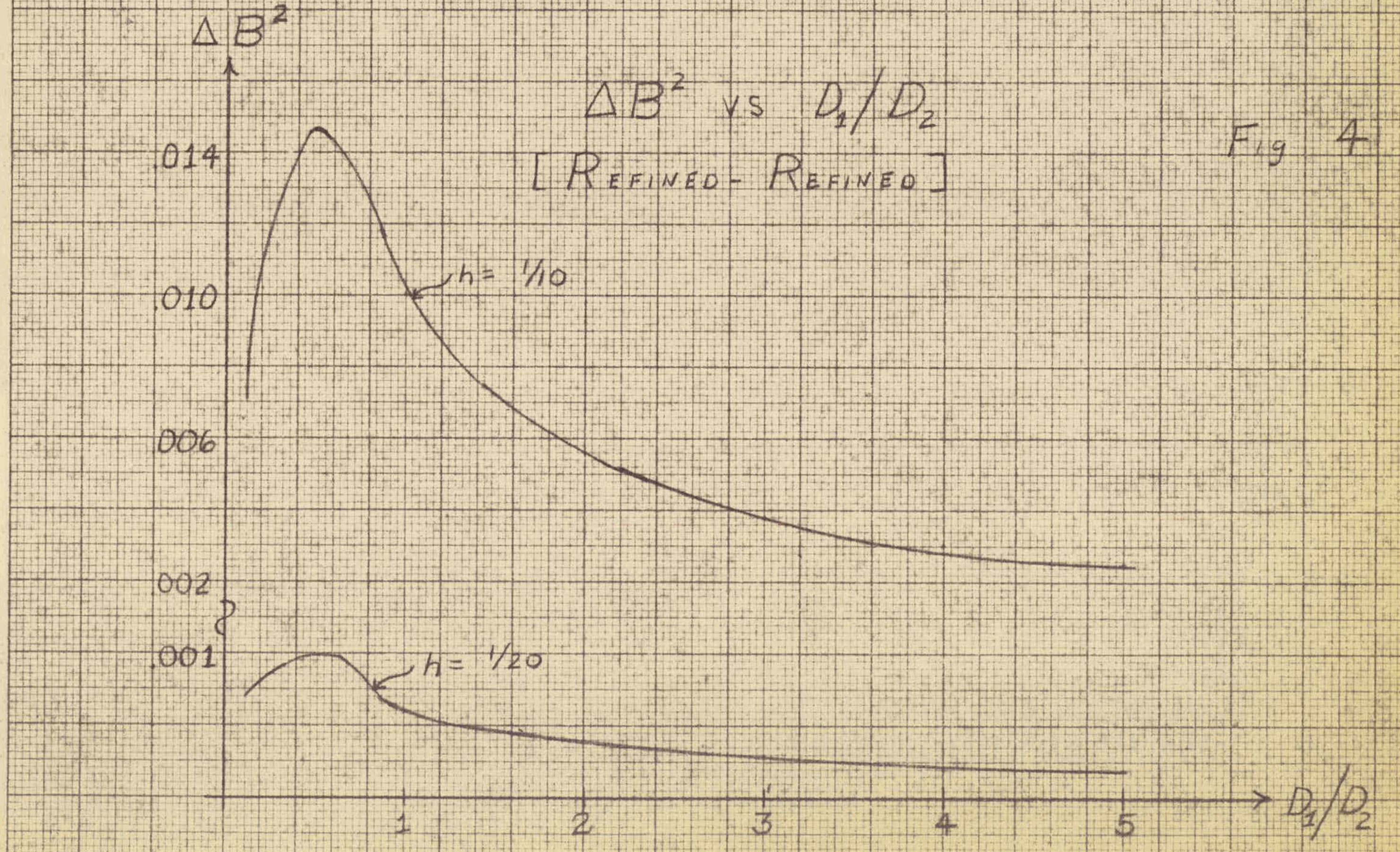

$-\Delta B^2$ vs D_1/D_2
[Crude - Crude]
$-\Delta B^2$
.5
.4
.3
.2
.1
1
2
3
4
5
D_1/D_2

Fig 2

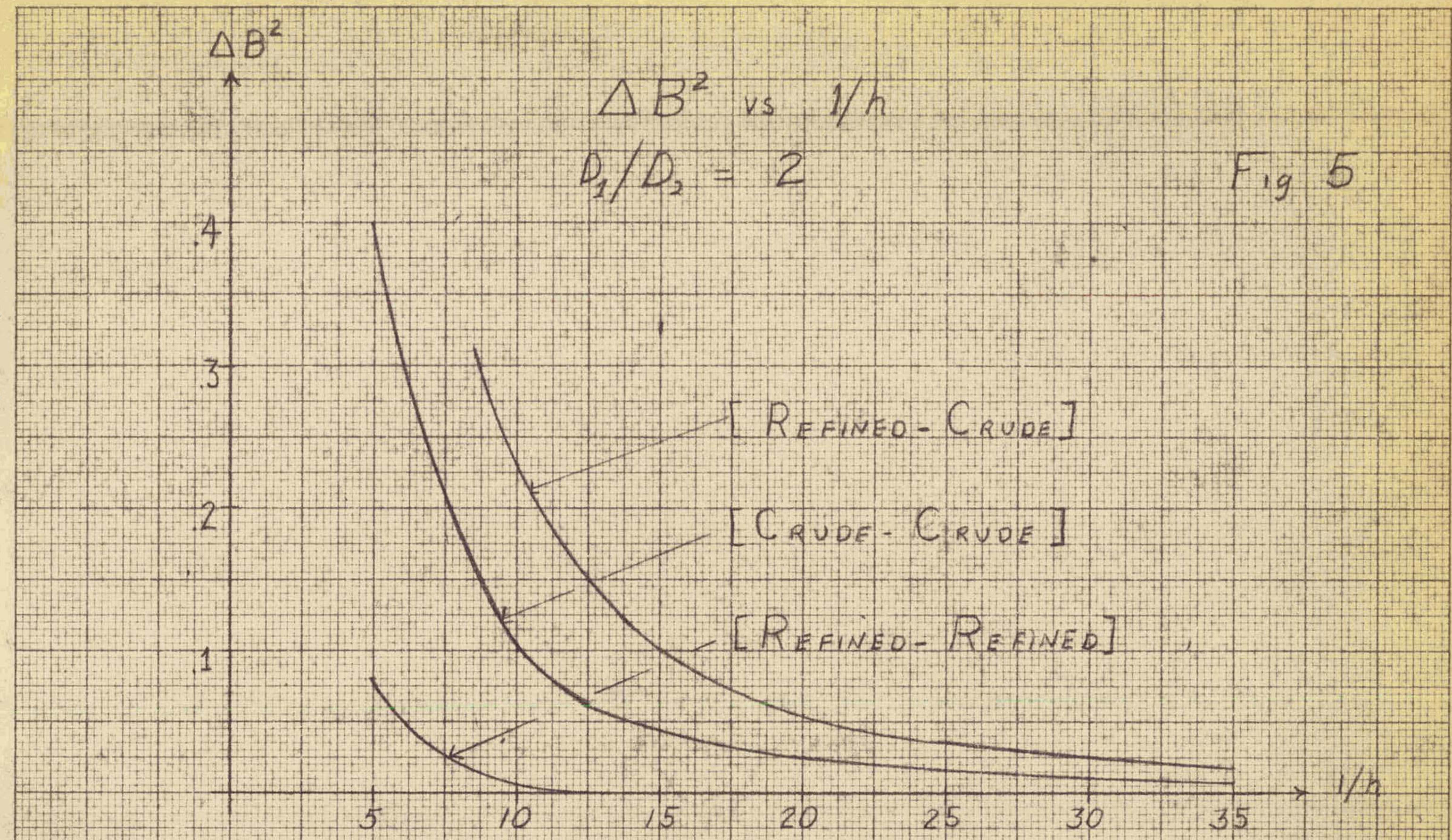


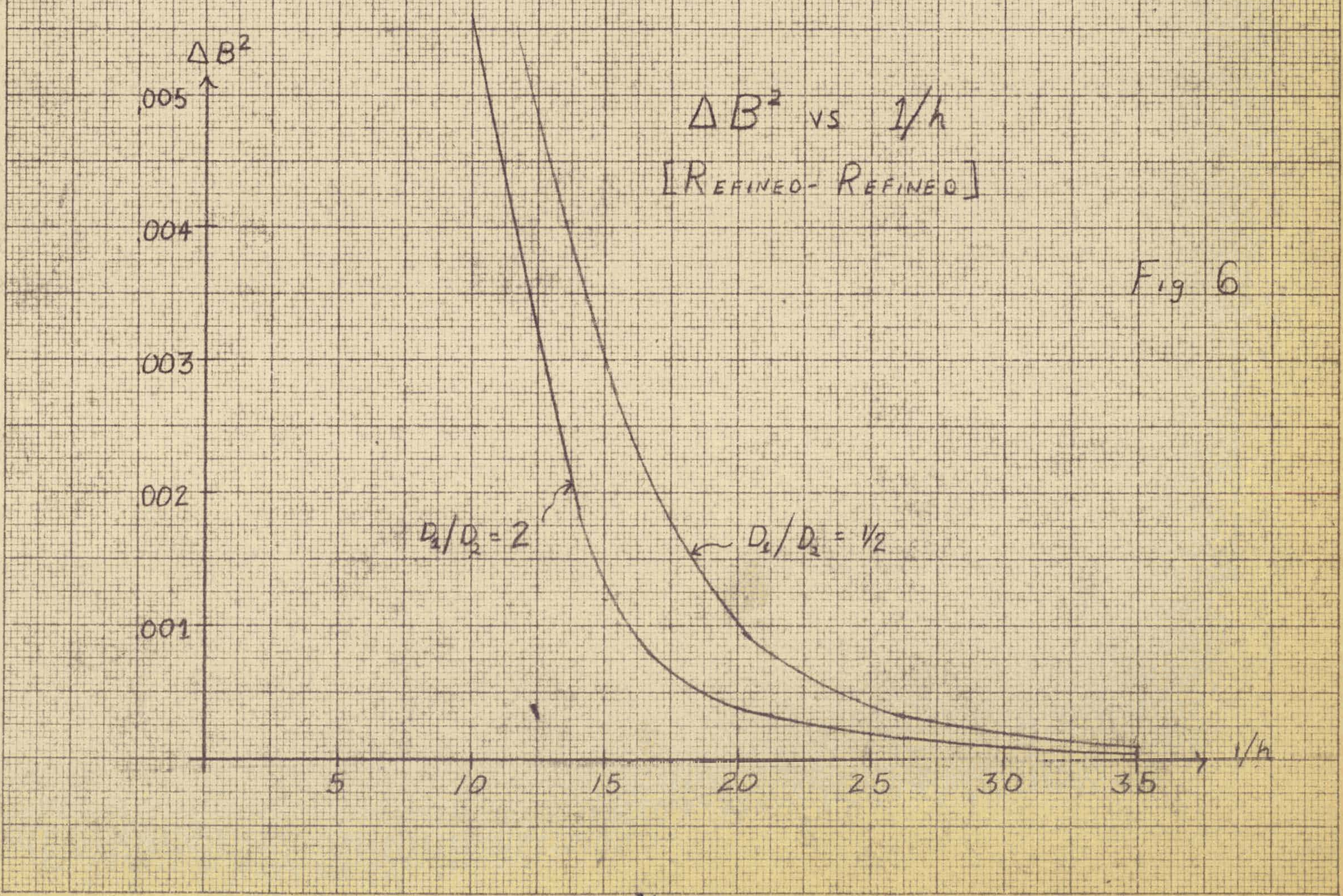
ΔB²
ΔB² vs D1/D2
[Refined - Crude]
Fig 3
h = 1/10
h = 1/20
.5
.4
.3
.2
.1
1
2
3
4
5
D1/D2



ΔB²
ΔB² vs D1/D2
[Refined - Refined]
Fig 4
h = 1/10
h = 1/20
.014
.010
.006
.002
.001
1
2
3
4
5
D1/D2

376 16


ΔB²
ΔB² vs 1/h
D₁/D₂ = 2
Fig 5
.4
.3
.2
.1
[Refined - Crude]
[Crude - Crude]
[Refined - Refined]
5
10
15
20
25
30
35
1/h


ΔB²
.005
.004
.003
.002
.001
ΔB² vs 1/h
[Refined - Refined]
Fig 6
D₁/D₂ = 2
D₁/D₂ = 1/2
5
10
15
20
25
30
35
1/h

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a-16

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