A Catalyst Falls Under a Little Poison Not Because Sites Are Lost but Because the Best Sites Go First

— In a model with **200000** sites, if every site has the same activity then poisoning a fraction θ leaves exactly $1-\theta$ (**0.500000** at $\theta = 0.5$) — the separator is whether the poison lands at random or takes the best sites first — [Paper 822]

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Abstract

A catalyst can lose much of its activity to a very small amount of poison.This paper counts, on a distribution of sites, that the fall cannot be explained by "sites were lost" and is decided by which sites go.No new theorem or law is claimed. First, with identical sites the effect follows the fraction——poisoning a fraction θ leaves exactly $1-\theta$ (0.500000 at $\theta = 0.5$) (Section 2). **Second, with spread activities but random poison, nothing changes——0.990156 against the uniform 0.990000 at $\theta = 0.01$** (Section 2). **Third, and this is the core. If the best sites go first, the same poison costs far more——0.943615 at $\theta = 0.01$, 0.799941 at 0.05, 0.669537 at 0.10 and 0.153309 at 0.50** (Section 3). **Fourth, the factor equals the share held by the top sites——the fall at $\theta = 0.01$ is 5.638529 times larger, the same number as the 0.056385 share of the top one percent** (Section 3). **Fifth, so "poison destroys active sites" is not enough——destroying the same number of sites gives results 5.638529 times apart** (Section 4). **Sixth, the separator is whether the poison lands at random or takes the best sites first——the shape of the fall says which is happening** (Section 4). **Keywords**: catalyst poisoning, active sites, non-uniform distribution, selective poisoning, remaining activity, model.

Scope of this paper (scope note): **No new theorem or law is claimed——catalyst poisoning, the non-uniformity of active sites, and large activity losses from small amounts of poison (selective poisoning) are all known.This is a model——200000 sites, activities drawn from an exponential distribution, and poison that merely removes a site.No real catalyst is discussed——particular materials, supports, poisons and regeneration procedures are not treated.The chemistry is not entered——adsorption equilibria, reaction mechanisms and temperature are not the subject.Diffusion is not treated——cases limited by diffusion in pores are not included; only the distribution of sites is examined.The numbers are model values——they come from the distribution and the order of removal, not from experiment.Relation to earlier papers**: **Paper 364 showed that selection alone raises the mean by 1.52 standard deviations and shrinks the spread to 0.45——this paper stands beside it: there the top is selected and kept, here the top is selected and destroyed, the same operation with the sign reversed.Paper 300 showed that whether two things share a root is decidable——"sites were lost" and "the good sites were lost" are distinct roots giving two falls from one amount of poison.**What is added is **setting uniform sites, random poison and selective poison on one footing**, **measuring the fall at $\theta = 0.01$ as 5.638529 times larger**, **confirming that this equals the 0.056385 share of the top one percent**, and **placing the separator on random versus best-first**.

1. Notation and the Question

Setting: **a catalyst carries 200000 sites, site i having activity a_i.Total activity is $\sum a_i$, and poisoning a fraction θ of the sites sets their activity to 0.**

$$\text{remaining share} = \frac{\sum_{i \notin P} a_i}{\sum_i a_i}, \qquad |P| = \theta N$$

Activities are set two ways, all equal or spread exponentially, and the poison two ways, at random or taking the most active first.

Question: **for the same amount of poison, how far apart can the remaining activity be?**

2. Uniform Sites and Random Poison

Computation 2.1: **with all activities equal, the remaining share was measured.**

poison fraction θ	remaining activity
0.01	0.990000
0.10	0.900000
0.50	0.500000

> **Observation 2.2**
>
> with identical sites the effect follows the fraction.The remaining activity is exactly $1-\theta$——here “sites were lost” and “activity fell” mean the same thing.

Computation 2.3: activities were spread exponentially and the poison applied at random.

poison fraction θ	uniform sites	spread sites, random poison
0.01	0.990000	0.990156
0.10	0.900000	0.899983
0.50	0.500000	0.500313

> **Observation 2.4**
>
> spread activities with random poison cannot be told apart.At $\theta = 0.01$ it is 0.990156 against 0.990000——chosen at random, good sites and poor sites go in the same proportion.

3. When the Best Sites Go First

Computation 3.1: the same sites were poisoned from the most active downwards.

poison fraction θ	uniform	random	best first
0.001	0.999000	0.999071	0.991985
0.010	0.990000	0.990156	0.943615
0.050	0.950000	0.950463	0.799941
0.100	0.900000	0.899983	0.669537
0.500	0.500000	0.500313	0.153309

Observation 3.2

this is the core. With the best sites going first, the same poison costs far more.At $\theta = 0.01$ the remaining activity is 0.943615, and the amount lost is 5.638529 times that of the uniform case——one percent of the sites were destroyed, but 5.6 percent of the work was lost.

Observation 3.3

the factor equals the share held by the top sites.The top one percent of sites hold 0.056385 of the total activity, the same number as the factor 5.638529——this is not a coincidence but a definition: destroying the top θ loses exactly the share the top θ holds.

4. The Separator

Observation 4.1

the separator is whether the poison lands at random or takes the best sites first.The same amount of poison leaves 0.990156 one way and 0.943615 the other——“poison destroys active sites” does not fix the fall until one says which sites.

Observation 4.2

the shape of the fall tells them apart.Increase the poison and watch whether the remaining activity follows the line $1 - \theta$ or drops steeply at first and then flattens——at $\theta = 0.5$, 0.500000 against 0.153309 cannot be mistaken.

Observation 4.3

placed beside Papers 364 and 300.Paper 364 showed that selection alone raises the mean——there the top is kept, here the top is destroyed, the same operation with the sign reversed.Paper 300 showed that sharing a root is decidable——"sites were lost" and "the good sites were lost" are distinct roots.

Observation 4.4

what is not said.Real catalysts, adsorption and mechanism, diffusion limitation and regeneration are not treated——what is shown is that the same amount of poison differs by 5.638529 times with the order of removal.

5. Census and Closing

1. **uniform at $\theta = 0.5$: $\mathbf{0.500000}$** (Computation 2.1): **following the fraction.**
2. **random at $\theta = 0.01$: $\mathbf{0.990156}$** (Computation 2.3): **same as uniform.**
3. **best first: $\mathbf{0.943615}$** (Computation 3.1): **the core.**
4. **$\mathbf{0.799941}$ at $\theta = 0.05$** (Computation 3.1): **a fifth gone.**
5. **$\mathbf{0.669537}$ at $\theta = 0.10$** (Computation 3.1): **a third gone.**
6. **$\mathbf{0.153309}$ at $\theta = 0.50$** (Computation 3.1): **far from 0.500000.**
7. **factor $\mathbf{5.638529}$** (Observation 3.2): **one percent of sites.**
8. **top one percent hold $\mathbf{0.056385}$** (Observation 3.3): **equal to the factor.**
9. **$\mathbf{0.991985}$ even at 0.001** (Computation 3.1): **a trace still bites.**
10. **random or best first** (Observation 4.1): **the separator; Papers 364, 300.**

Closing: **A catalyst falls under a little poison not because sites are lost but because the best sites go first.With identical sites the remaining activity is exactly $1 - \theta$, and with spread activities under random poison it is 0.990156**

against 0.990000 at $\theta = 0.01$, indistinguishable——chosen at random, good and poor sites go in the same proportion.But with the most active going first it is 0.943615 at $\theta = 0.01$, 0.799941 at 0.05, 0.669537 at 0.10 and 0.153309 at 0.50, a fall 5.638529 times larger at $\theta = 0.01$, equal to the 0.056385 share held by the top one percent ——destroying the top θ loses exactly the share the top θ holds.The separator is whether the poison lands at random or takes the best sites first.Placed among the earlier papers——standing beside Paper 364's "selection alone" (there the top is kept), and keeping Paper 300's discipline between losing sites and losing the good sites.To be honest—— these are values from a model with an exponential distribution, not from a real catalyst or from diffusion.

References

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