**Socratic Prompting with Argo: Assessment**

Michael Stuhr (CSE, Chemical Dynamics Group)

**Original Prompt:**

“For multi-channel thermal decomposition reactions, how can reaction channels with high-energy transition states have higher branching fraction than reaction channels with low-energy transition states?”

**Socratic Reformulation:**

“What factors could lead to a reaction channel with a high-energy transition state having a higher branching fraction than one with a low-energy transition state, and how might these factors challenge our typical understanding of reaction dynamics?”

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| **Principles** | **(Follow-Up) Prompts** |
| **Dialectic** | **Original Prompt:**  “For multi-channel thermal decomposition reactions, how can reaction channels with high-energy transition states have higher branching fraction than reaction channels with low-energy transition states?” |
| **Generalization** | **Follow-up Prompt 1:**  “Are there known examples where high-energy pathways are favored in chemical reactions, and how might these examples help us generalize principles about reaction dynamics?” |
| **Induction** | **Follow-up Prompt 2:**  “What general principles can we derive from these examples about the factors that influence reaction pathway selection, and how might these principles be reconciled with traditional views of reaction kinetics and thermodynamics?” |
| **Elenchus** | **Follow-up Prompt 3:**  “Are there any contradictions or surprising outcomes in reactions under kinetic control that challenge traditional kinetic models, and how might analogies to other systems help us generalize these findings?” |

1. **Motivation**

*Why is this problem important in chemistry/materials science?*

The branching of competing reaction channels in unimolecular decomposition of molecular species in the gas phase can show a complex dependence on temperature and pressure. For example, while low-energy pathways through tight transition states may dominate at low temperatures, a high-energy channel with a loose transition state can become increasingly competitive as the temperature increases and even take over as the main decomposition channel. This effect, which is called channel switching, is well known in the field of reaction kinetics and can be explained by the energy (*E*) and angular momentum (connected to the rotational quantum number *J*) dependencies of the specific rate constant *k*(*E*,*J*) for the two different transition state geometries. Channel switching can have a profound effect on the overall product distribution of the studied reaction and subsequent chemistry.

*What challenges exist in solving this problem using traditional LLM approaches?*

While channel switching is a well-established concept in reaction kinetics (transition state theory), unguided prompting of LLMs is expected to result in ‘textbook-style’ responses that focus on the more general effects of temperature (and other parameters) on rate constants. Ideally, the model responses should specifically address the original user question, which is related to the relationship between transitions states and the branching fractions of the corresponding reaction channels.

*How could a structured Socratic approach improve reasoning and outcomes?*

By using a Socratic (guided) prompting approach, the model responses can be steered towards more refined responses that are more likely to guide the user to the topic of transition state geometry and channel switching, which are more useful for answering the posed question than more general concepts.

1. **The Mixed Socratic Prompt Method Used**

For this problem, I assumed a hypothetical user asking for an explanation for the (perhaps initially unintuitive) observation of favorable high-energy reaction pathways (**Dialectic**). I proceeded with **Generalization, Induction,** and **Elenchus**, because the suggested follow-up prompts seemed to be the most promising for extracting a useful answer to the question. More specifically, Follow-up Prompts 1 was used to encourage the model to restate the key factors for channel branching. Likewise,Follow-up Prompt 2 aimed to induce reconsideration and refinement of previous statements made by the model. Many alternative follow-up prompts strayed too far from the original issue to be considered (see transcript).

1. **What Are the Prompts Used?**

***Original Prompt:***

“For multi-channel thermal decomposition reactions, how can reaction channels with high-energy transition states have higher branching fraction than reaction channels with low-energy transition states?”

***Socratic Reformulation:***

“What factors could lead to a reaction channel with a high-energy transition state having a higher branching fraction than one with a low-energy transition state, and how might these factors challenge our typical understanding of reaction dynamics?”

1. **What Are the Outcomes of This Example?**

*How did the LLM refine its answers over iterations?*

In the first answer, the model guided by Socratic prompting correctly identified density of states in the transition state, which is directly related to specific rate constant *k*(*E*,*J*) mentioned above, as an important factor in transition state theory. However, neither the initial model response nor the following iterations mentioned transition state geometry (loose vs. tight), *E*- and *J*-dependence of *k*, or channel switching. Although a useful overview of various aspects relevant to reaction kinetics was provided, it would be difficult for the hypothetical user to find an appropriate answer to their initial question. Follow-up Prompt 1was supposed to refine the model response by asking for specific examples and generalizations. However, the model switched its focus to kinetic vs. thermodynamic control instead, which was not mentioned in the first answer and is only indirectly related to the original question. In general, many model responses included vague or irrelevant statements, e.g., “A high-energy transition state might lead to a higher branching fraction […] if it is part of a more favorable kinetic pathway.” Obviously, the point of the initial prompt was to explain *why* a high-energy pathway can be more favorable.

*What key insights or discoveries emerged?*

Guided by the Socratic prompting approach, the model provided generally useful pointers to key concepts in reaction kinetics. It seems to be difficult to prevent the model from going off track, although this issue is much worse for the non-Socratic approach. It is entirely possible that the initial question is too specific. Moreover, user-written follow-up prompts may have led to better responses for the example described here.

*Any unexpected results or challenges?*

Some test runs with alternative initial prompts on the same original question (not shown here) suggest that both the Socratic reformulation and the suggested follow-up prompts are highly dependent on the specific phrasing of the initial prompt and the terms used therein. This may limit the ability of the Socratic approach to refine model behavior, depending on the original user input. It seems likely that the Socratic reformulation step has a significant effect on model response, since this process introduces new Socratic elements for the provided prompt.

1. **Comparison to a Non-Socratic Approach**

*How did reasoning depth, self-correction, and hypothesis refinement compare?*

The conventional approach led to more shorthand ‘bullet point’ responses with shallower statements and fewer explanations. Further refinement of these results by using follow-up prompts seemed to be minimal. In contrast, the Socratic approach led to a more ‘conversational’ and responsive experience with significantly fewer points being restated.

*Would a traditional direct-answer prompt have produced different results?*

Non-Socratic prompting with the same initial question led to much more formulaic statements that seemed too unspecific to ultimately lead to a useful answer to the problem at hand.

*Did the Socratic method improve clarity, adaptability, or accuracy?*

Overall, the Socratic prompting approach provided clearer statements and more specific points. In my opinion, this method has led to more useful responses that can be applied more easily.