# Functional Contradictions: Insights into Process Improvement

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Process intensifications are a critical part of process development in the chemical process industries (CPI). In addition to traditional approaches, identifying and resolving contradictions can bring about new and valuable process improvements.

As engineers working in the chemical process industries (CPI), our mantra is to find ways of making things "faster, better, cheaper." This expression is well-known and was used often by Daniel Goldin, administrator of the National Aeronautics and Space Administration (NASA) from 1992 to 2001. To clarify, faster means more output in a defined time period (or the same output in less time); better means improved safety, quality, and sustainability; and cheaper means at lower capital and operating cost.

These objectives align well with current thinking about process intensification (PI). In 2015, the U.S. Dept. of Energy (DOE) ran a two-day workshop on process intensification *(1)*. The report from this workshop defines PI as breakthroughs that lead to significant improvements in performance. The report outlines areas of opportunity such as thermal intensification, mixing and mass transfer, chemical separation and crosscutting technologies, and other opportunities.

## Process intensification via contradictions

One approach to process intensification is to look for contradictions within the chemical process *(2)*. A contradiction occurs when one action produces a useful result but also a harmful effect. For example, a chemical reaction may proceed at a higher rate if the temperature is increased, but the higher temperature also produces more unwanted byproducts.

Genrich Altshuller, an engineer in the former Soviet Union, studied contradictions extensively during the 1940s. In his studies, Altshuller observed that processes of many kinds were fundamentally limited by contradictions. This is because a contradiction implies a compromise. In a chemical reaction, the incremental value of the additional product obtained as a result of a slight temperature increase could more than compensate for the lower yield caused by producing more unwanted byproducts. Further temperature increases would reach a point of diminishing returns, where the temperature increase diminishes value. In such cases, engineers use an approach like Six Sigma to find the optimum operating point, a compromise between the benefits and harm of increasing temperature. If the compromise is avoided (*e.g.*, an increase in temperature would not detract from the yield), the contradiction is resolved.

### Function modeling

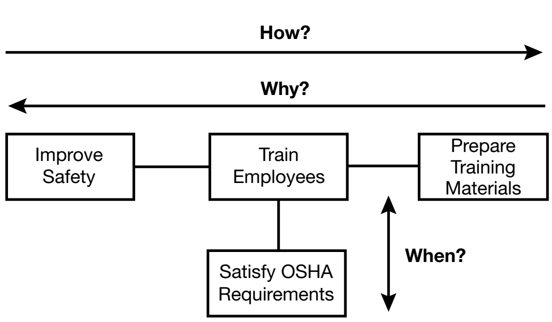
Modern chemical plants, petrochemical plants, and refineries are typically large complex operations. The number of areas and unit operations for potential improvement can be overwhelming. Identifying process improvement opportunities requires a systematic approach to manage and prioritize areas that offer significant performance improvements.

During World War II, labor, materials, and component parts were scarce and delays in manufacturing were common. Lawrence Miles, Jerry Leftow, and Harry Erlicher, engineers at General Electric (GE), recognized that substitutes could be used as long as the substitute performed essentially the same function as the original. In other words, it is not important what something is but rather what it does. This became known as function analysis.

Charles Bytheway, another GE engineer, developed a graphical technique to map the functions in a system and show their relationships. Bytheway's approach is called the function analysis system technique (FAST). FAST diagrams show how, why, and when processes occur in a system *(3)*.

In a FAST diagram (Figure 1), the leftmost function is the primary function — it describes the desired action to be performed. Starting with the primary function, move to the right and ask: How is this function performed? Continue going from left to right asking "how?" The logic of the model is validated by moving from right to left and asking: Why is this function performed? Completing the how-why logic forms the primary logic path. Once the primary logic path is complete, examine each function and ask: When this function is performed, are there any consequential functions?

In the example in Figure 1, the primary function, improve safety, is on the left. Going from left to right, ask and answer a series of "how" questions: How do you improve safety? The answer is the connected function: train




▲ **Figure 1.** This sample FAST diagram describes the how, why, and when relationships associated with the primary function "improve safety."

Once the primary how-why logic path is complete, examine each function and ask: When this function is performed, are there any consequential functions?

employees. How do you train employees? The connected function to the right explains: by preparing training materials.

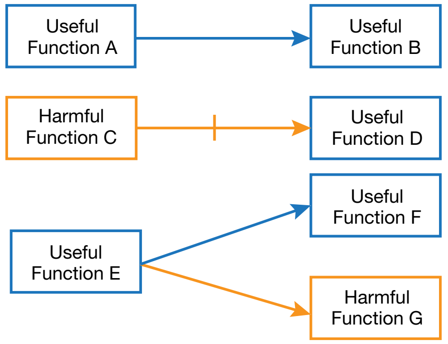
The logic in the model can be validated by going from right to left and asking "why?" So, why do you prepare training materials? To train employees. And, why do you train employees? To improve safety.

Examine each function and ask: When this function is performed, are there any consequential functions? In this case, when you train employees, you satisfy U.S. Occupational Safety and Health Administration (OSHA) requirements.

FAST diagrams are limited in their ability to identify contradictions in chemical processes. First, the rigid structure can become overly complex when modeling large processes. To simplify the diagram, connect functions with arrows. When moving against the direction of the arrow, ask "how?" When moving in the direction of the arrow, ask "why?"

Second, FAST diagrams make no distinction between useful and harmful functions. Recall that a contradiction occurs when one action (useful function) produces a useful result (useful function) but also a harmful effect (harmful function). Therefore, it is helpful to make a visual distinction between useful and harmful functions in the function model. To do this, add a crosshatch to an arrow to indicate counteraction.

Figure 2 summarizes these modifications to the traditional FAST diagram. The useful Function A produces the useful Function B, as indicated by the connecting arrow. The same how-why logic is applied here. One function can

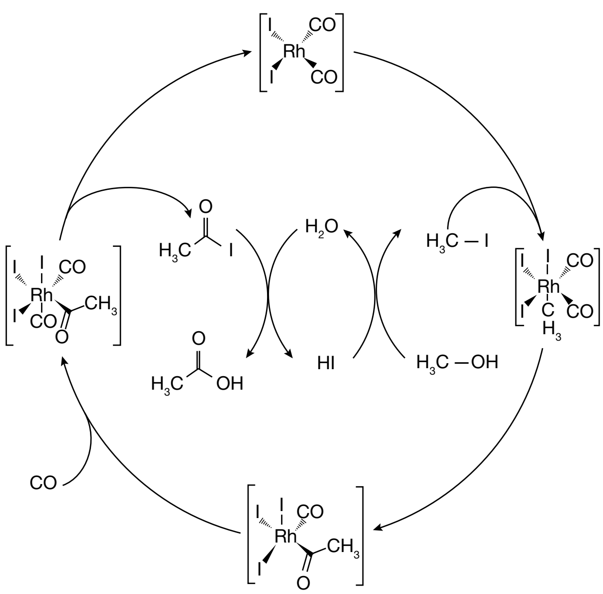



▲ **Figure 2.** The FAST diagram can be modified to make it easier to understand. Useful functions are outlined in blue, while harmful functions are outlined in orange. Moving against the direction of the arrow ask "how?" Moving in the direction of the arrow ask "why?"

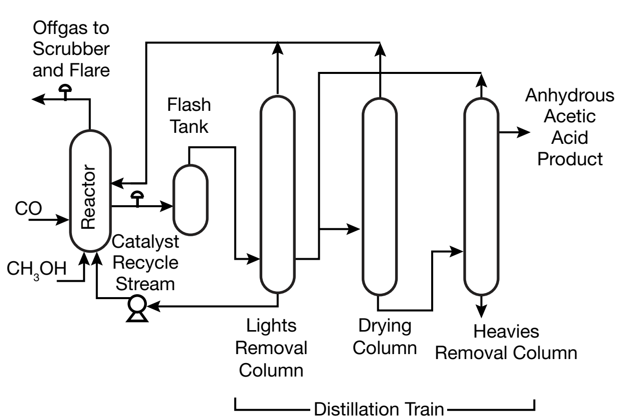
counteract another. In this case, harmful Function C counteracts useful Function D, as indicated by the crosshatched arrow. A contradiction occurs when a useful function produces a useful result as well as a harmful effect. In this example, useful Function E produces useful Function F, but it also produces harmful Function G.

### Function modeling example: Methanol carbonylation

Acetic acid ($CH_3COOH$) is commonly produced by the catalytic carbonylation of methanol ($CH_3OH$) *(4)*. This process was originally developed by BASF and commercialized by Monsanto in 1966. The carbonylation reaction involves insertion of carbon monoxide (CO) into the C-O bond in the methanol:



▲ **Figure 3.** Acetic acid is produced by the catalytic carbonylation of methanol.




▲ **Figure 4.** The methanol carbonylation process uses a reactor, a flash tank, and three distillation columns to produce anhydrous acetic acid.

$$CH_3OH + CO \rightarrow CH_3COOH$$

The catalytic system (Figure 3) *(5)* involves a transition metal catalyst, typically a rhodium complex, and a methyl iodide ($CH_3I$) cocatalyst:

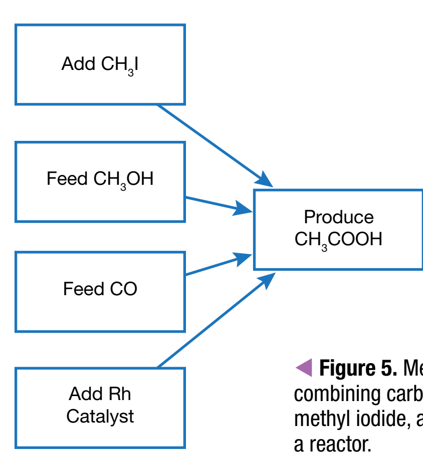
$$CH_3OH + CH_3COOH \rightarrow CH_3COOCH_3 + H_2O$$
$$CH_3COOCH_3 + HI \rightarrow CH_3I + CH_3COOH$$
$$CH_3I + CO \rightarrow CH_3COI$$
$$CH_3COI + H_2O \rightarrow CH_3COOH + HI$$

In this process, excess water is required to stabilize the catalyst and prevent precipitation of the rhodium salts. The original Monsanto process used water levels around 15%. The presence of water stabilizes the catalyst, but it also has several negative effects. One negative effect is that the water must be removed from the product to produce the desired anhydrous product form. This involves a highly energy intensive distillation process. In addition, water ionizes hydrogen iodide, so the reactor contents become highly corrosive. To avoid this, much of the equipment must be made from corrosion-resistant materials, which increases capital cost. Another disadvantage of the presence of water is that water and CO react in the water-gas-shift reaction:

$$H_2O + CO \rightarrow CO_2 + H_2$$

This reaction reduces the CO feedstock and produces $CO_2$ as a byproduct.

Figure 4 is a schematic diagram of a methanol carbonylation plant. The products leaving the reactor enter a flash tank; water, acetic acid, and lighter components go overhead and heavier components are recycled to the reactor. Without the presence of water, a higher concentration of catalyst in the bottom of the flash tank causes it to precipitate out of solution. The lights removal column removes methyl iodide and components lighter than methyl iodide,




◀ **Figure 5.** Methanol is produced by combining carbon monoxide, methanol, methyl iodide, and a rhodium catalyst in a reactor.

which are recycled to the reactor. The drying column removes water and products that are heavier than water, like propionic acid.

## Use functional models to find contraditions

The first step in finding a contradiction is building a function model of the primary logic path. In the case of methanol carbonylation, an examination of the basic chemistry reveals the logic. Figure 5 is the function model for this process. Following the how-why approach, ask: How is acetic acid produced? Answer: by feeding methanol to the reactor, feeding CO to the reactor, adding methyl iodide as a promoter, and adding a rhodium catalyst. A more detailed model of the chemistry is possible, but it is often useful to start simple and add detail later if needed.

Next ask: When these functions are performed, are there any consequential functions? Low water levels in the reactor cause the catalyst to precipitate, which counteracts the effectiveness of the rhodium catalyst. To counteract the rhodium precipitation, excess water is added to stabilize the catalyst. The excess water also has some harmful effects that must be considered. Because the acetic acid product is sold in the anhydrous form, the water must be removed, which consumes energy and increases cost. The excess water also forms a highly acidic solution with the hydrogen iodide in the reactor, which corrodes the equipment. To counteract the corrosion, the reactor is made of zirconium, which increases the cost to build the plant. Finally, the excess water produces the water-gas shift reaction, which consumes CO feed and increases operating costs. Figure 6 depicts these consequential effects.

The function "Add Excess Water" is said to be in contradiction. It produces the benefit of stabilizing the catalyst, but it also produces three harmful functions (it removes water, ionizes the hydrogen iodide, and produces a water-gas shift) that increase production costs. So, is the presence of water beneficial in the reactor? The answer is both yes and no.

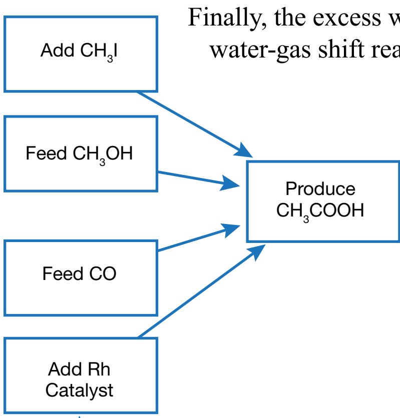
One approach to address the problem of water in the reactor is to find a way to minimize the need for excess water. An example of this is the Hoechst-Celanese acid optimization technology *(6)*. Iodide salt promoters allow carbonylation to be carried out at lower water levels than the original Monsanto design. Water levels can be reduced from around 15% to less than 5%. Methyl acetate concentration increases, which reacts with other components:

$$CH_3COOCH_3 + LiI \rightarrow CH_3I + LiOCOOCH_3$$
$$LiOCOOCH_3 + HI \rightarrow LiI + CH_3COOH$$

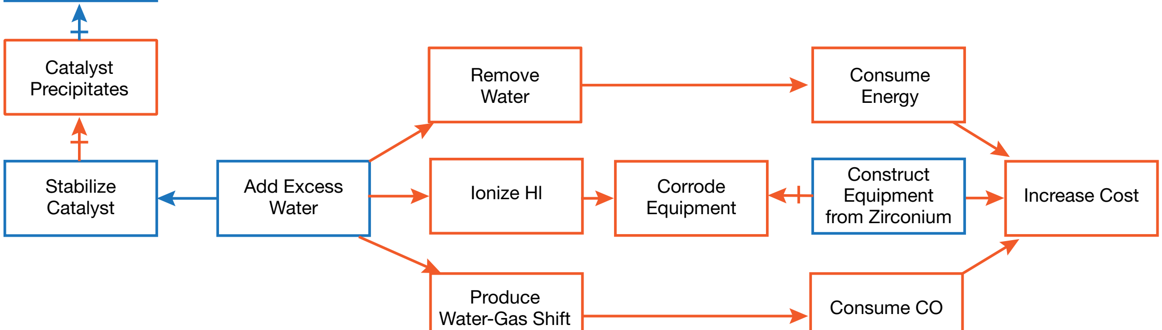
In this case, the contradiction surrounding the use of excess water still exists, but has less impact.

A better approach would be to resolve or eliminate the contradiction, thereby removing the need for any compromise. In many cases, taking a closer look at the how-why-when relationships in the function model can spur new ideas.

Consider the how-why relationship between adding excess water and stabilizing the catalyst. The logic appears correct. How is the catalyst stabilized? By adding excess water. And, why is excess water added? To stabilize the catalyst. But is this an adequate explanation of exactly how and why this happens?




▼ **Figure 6.** The useful function "Add Excess Water" produces the useful function "Stabilize Catalyst," but it also produces three harmful functions: "Remove Water," "Ionize HI," and "Produce Water-Gas Shift." The function "Add Excess Water" is said to be in contradiction because it produces both useful and harmful functions.

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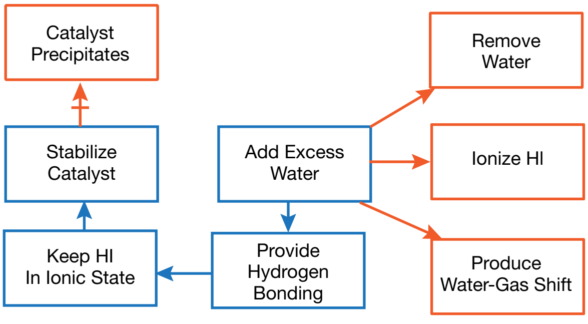
Further study of the mechanism of stabilization produced the expanded functional relationships in Figure 7. The purpose of water is to enable hydrogen bonding. The hydrogen bonding properties of water keep the hydrogen iodide in an ionic state. The ionization of the hydrogen iodide works to keep the rhodium catalyst in the +1 valence state, which is the active form of the rhodium salt needed for catalytic activity.

One solution to the excess water problem is to replace the water with another compound that performs the same function as water, namely hydrogen bonding, but at a higher boiling point than acetic acid. Recall that water evaporates in the flash tank because it has a lower boiling point than acetic acid. If hydrogen bonding is facilitated by a compound with a higher boiling point, then there will be no need to add water or to remove the water from the finished product. Hydrogen iodide will not be ionized in the presence of water and there will be no water-gas shift reaction to consume CO feed. Potential hydrogen bonding additives include sulfones ($R^3SO_2R^4$), and sulfone-containing oligomers, co-oligomers, polymers, and copolymers *(7)*.

## Resolving contradictions

Based on his insights into contradictions, Altshuller developed systematic methods to resolve contradictions. This body of work is known as TRIZ, the Russian acronym for Theory of Inventive Problem Solving. A previous three-part article in *CEP (8–10)* covered the basics of TRIZ and its applications. In general, contradictions are resolved by performing a separation in state such that in State 1, the useful result is produced, and in State 2, the harmful effect is counteracted. Furthermore, there are four categories of separation in state: space, time, structure, and upon a condition. The left side of Figure 8 shows a typical contradiction between Functions A, B, and C. The contradiction is resolved when Function A is separated into two states, as indicated by the vertical arrow between Function A1 and Function A2.



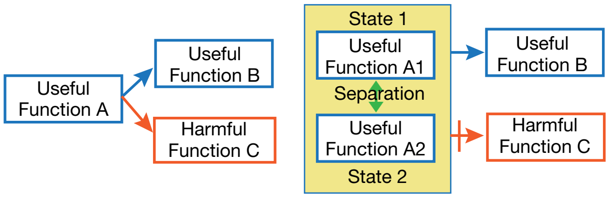

▲ **Figure 7.** Expanding the function model shows how water stabilizes the catalyst. The hydrogen bonding properties of water keep hydrogen iodide in an ionic state.

Separation in space illustrates a function that occurs in one location and not in another location. For example, many people need one prescription for glasses to see things far away and a different prescription to see things up close. A compromise solution would be one lens that would allow the user to see things a little fuzzy far away and also a little fuzzy up close. Or, carry two pairs of glasses and change as needed. Neither of these solutions is ideal. Bifocals resolve the contradiction. In one location, the top part of the lens, the prescription allows one to see things far away. In another location, the bottom part of the lens, the prescription allows one to see things up close. Bifocals are an example of resolving a contradiction by separation in space.

Separation in time defines a function that exists during one time period and not during another time period. In designing an aircraft, a large wing area enables the plane to fly at low speeds, which is beneficial for takeoff and landing. However, when cruising at high speed, a large wing area creates drag. Aircraft such as the F-15 have movable wings that can be extended to increase wing area during times when the plane is taking off or landing or needs to maneuver sharply, and then the wings can be retracted to reduce drag from the wing area when the plane is traveling at high speed. Moveable wings on aircraft are an example of resolving a contradiction by separation in time — the wing area can be large during one time period and can be small during another time period.

Separation in structure describes a function that exists at the system level but does not exist at the subsystem level, or vice versa. On a sailboat, a narrow beam will make the boat fast. But the narrow beam will also make the boat unstable and vulnerable to tipping. A catamaran effectively resolves this contradiction by performing a separation in structure. The beam of a catamaran at the system level (the width of the entire boat) is very broad. The beam at the subsystem level (each individual hull) is very narrow.

Separation upon a condition defines a function that is present under one condition but not under another condition. Lighting creates a safe environment for someone



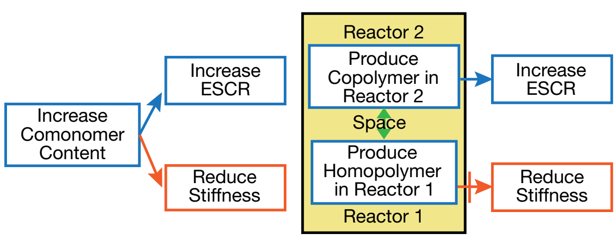

▲ **Figure 8.** Contradictions are resolved by separating the function that produces the contradiction (Function A) into two states. In State 1, the useful result (Function B) is produced, and in the State 2, the harmful effect (Function C) is counteracted.

entering a restroom. But when the restroom is vacant, keeping the lights on wastes energy. This contradiction can be resolved with a separation upon condition. The first condition is when someone is in the restroom, and the second condition is when the restroom is vacant. A motion sensor can be used to switch lights on when someone enters the restroom and switch them off when the restroom is vacant.

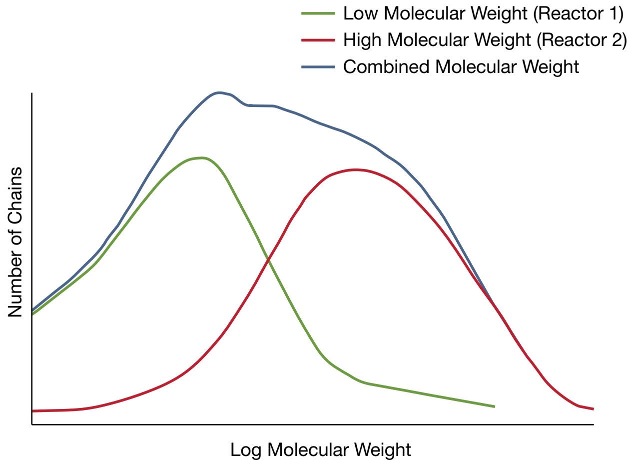
### An example in copolymers

High-density polyethylene (HDPE) copolymer resins are commonly used to make blow-molded bottles. Liquids such as detergents can cause environmental stress cracks in the bottles known as crazing, and some chemicals can accelerate polymer crazing, especially at locations under stress such as sharp corners. Using a copolymer such as an ethylene/1-hexene copolymer can increase the environmental stress crack resistance (ESCR). However, the addition of 1-hexene reduces polymer density and stiffness. Bottles require a minimum amount of stiffness to keep it upright and intact, especially when several cases of bottles are stacked. Making the bottles from HDPE homopolymer would provide excellent stiffness but very poor ESCR. Figure 9 illustrates this contradiction.

A separation in space — using two reactors — can resolve this contradiction *(11)*, as shown in Figure 9. Instead of conducting the reaction in one location (one reactor), the reaction can be conducted in two different locations (two reactors). The first reactor produces




▲ **Figure 9.** Increasing the concentration of comonomer in a high-density polyethylene copolymer improves the environmental stress crack resistance (ESCR). However, the increased comonomer also reduces polymer stiffness. The use of two reactors resolves the contradiction between the high-density polyethylene copolymer's stiffness and its resistance to environmental stress cracking.




▲ **Figure 10.** HDPE copolymer produced in two reactors has a bimodal molecular weight distribution, representing a separation in structure.

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## Additional Resources


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homopolymer HDPE. The resin is then transferred to the second reactor, where more ethylene and comonomer are added to produce a high comonomer fraction within the HDPE homopolymer structure.

Interestingly, this resolution can also be viewed as a separation in time or a separation in structure. It is a separation in time because the homopolymer reaction runs during the first time period and the copolymer reaction in the second time period. It is a separation in structure because the two-reactor process produces a resin with a bimodal molecular weight distribution. The combined molecular weight is the distribution of the entire system, while at the subsystem level there are two separate molecular weight distributions (Figure 10) *(12)*.

A resolution can be seen as a separation in more than one way. This is because a problem and its solution can often be looked at in more than one way. However, the form of the solution is not important, as long as an innovative solution that resolves the contradiction is determined. In this case, the method is less important than the resolution itself.

## Closing thoughts

Function models help identify contradictions that limit process performance. Many times contradictions are viewed as intractable. However, resolving a contradiction is possible once the true nature of the contradiction is understood. Questioning the how-why-when logic in a function model assists in a more fundamental understanding of the chemical and physical phenomena occurring in a process. The process of building function models creates a common understanding of how processes operate and where opportunities for improvement lie. CEP

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