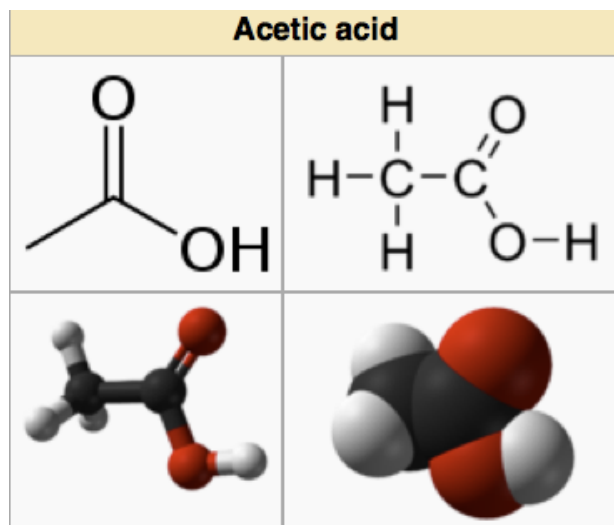# *Using TRIZ for Innovation and Patent Design in the Chemical Industry*



By
Peter Hanik

Presented at
TRIZCon2011

pretium innovation
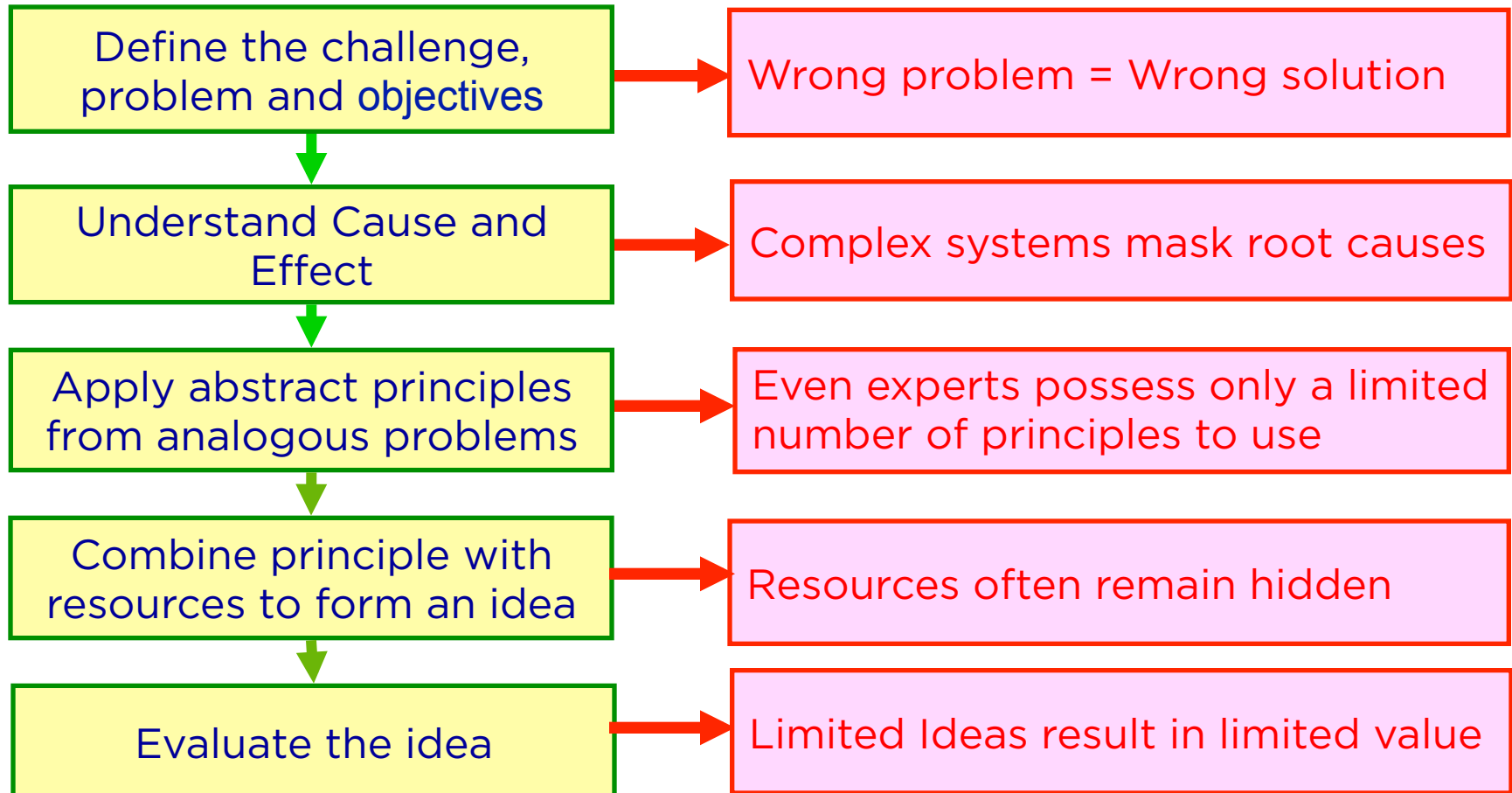
# *The Innovation*

Reduce the operating and capital cost to produce acetic acid via methanol carbonylation

# *The Intuitive Innovator*

## The Intuitive Process...        ...and its limitations

| The Intuitive Process | ...and its limitations |
|---|---|
| Define the challenge, problem and objectives | Wrong problem = Wrong solution |
| Understand Cause and Effect | Complex systems mask root causes |
| Apply abstract principles from analogous problems | Even experts possess only a limited number of principles to use |
| Combine principle with resources to form an idea | Resources often remain hidden |
| Evaluate the idea | Limited Ideas result in limited value |

# *Function Modeling*

# *Function Modeling*

Function A

Functions can be useful

Function B

Functions can be harmful

Function C ──▶ Function D

One function can produce another

Function E ──◇ Function F
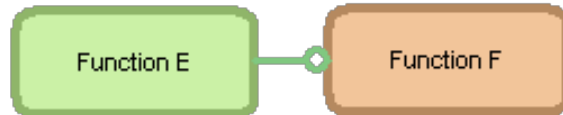
One function can counteract another

Function H
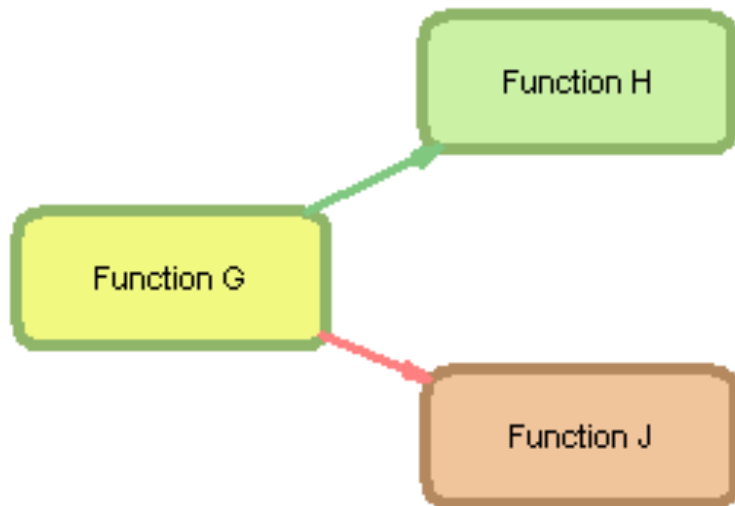
Function G
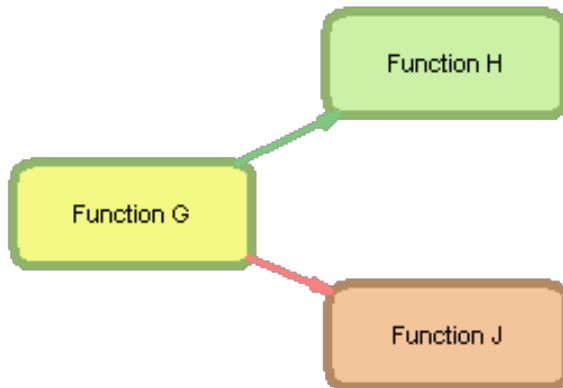
Function J

A contradiction exists when a function produces a useful result and also produces a harmful result

# *Three Opportunities for Improvement*

There are only three ways to improve system performance – improve the sum of useful functions, reduce the sum of harmful functions and resolve the contradictions.



1. Find a way to improve Function H.

2. Resolve the contradiction: Function G should produce Function H, and should not produce Function J.

3. Find a way to counteract Function J.

# *Ideality*

$$\text{Ideality} = \frac{\text{Sum of Useful Functions}}{\text{Sum of Harmful Functions}} \longrightarrow \infty$$

**Primary Function of a Paper Clip = Hold Two Pieces of Paper Together**
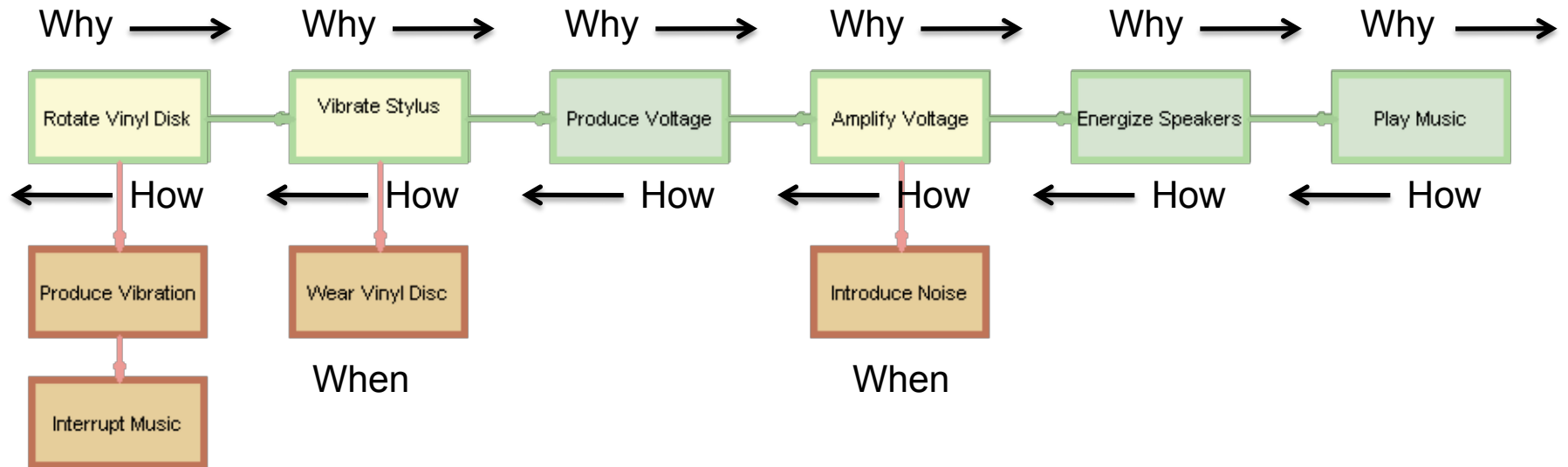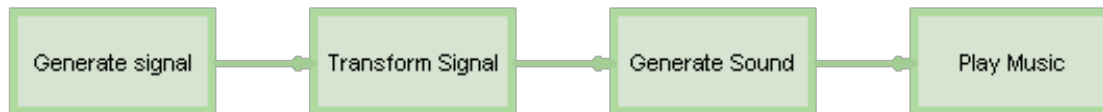**Ideal Vision = Papers held together without the Paper Clip Existing**
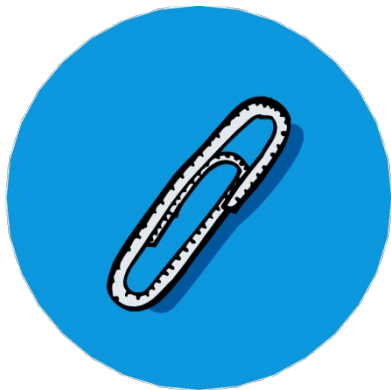
| Good | Better | Nearly Ideal |
| :---: | :---: | :---: |

# *Function Modeling*

## Phonograph Function Model

Why ➝  Why ➝  Why ➝  Why ➝  Why ➝  Why ➝

| Rotate Vinyl Disk | Vibrate Stylus | Produce Voltage | Amplify Voltage | Energize Speakers | Play Music |

← How  ← How  ← How  ← How  ← How  ← How

| Produce Vibration | Wear Vinyl Disc | | Introduce Noise | | |

When                              When

| Interrupt Music |

When

## Pure Function Model

| Generate signal | Transform Signal | Generate Sound | Play Music |

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# *Evolution of Functionality*
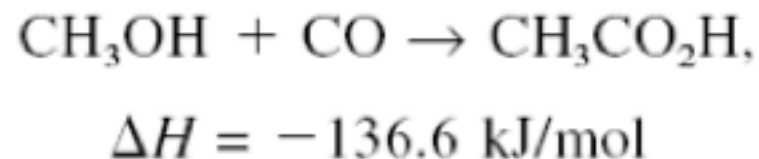
"Play Music"
Functionality Delivered



Increasing Ideality

# Function Modeling Acetic Acid

# *Simple Process Function Model*



$$CH_3OH + CO \rightarrow CH_3CO_2H,$$

$$\Delta H = -136.6 \text{ kJ/mol}$$
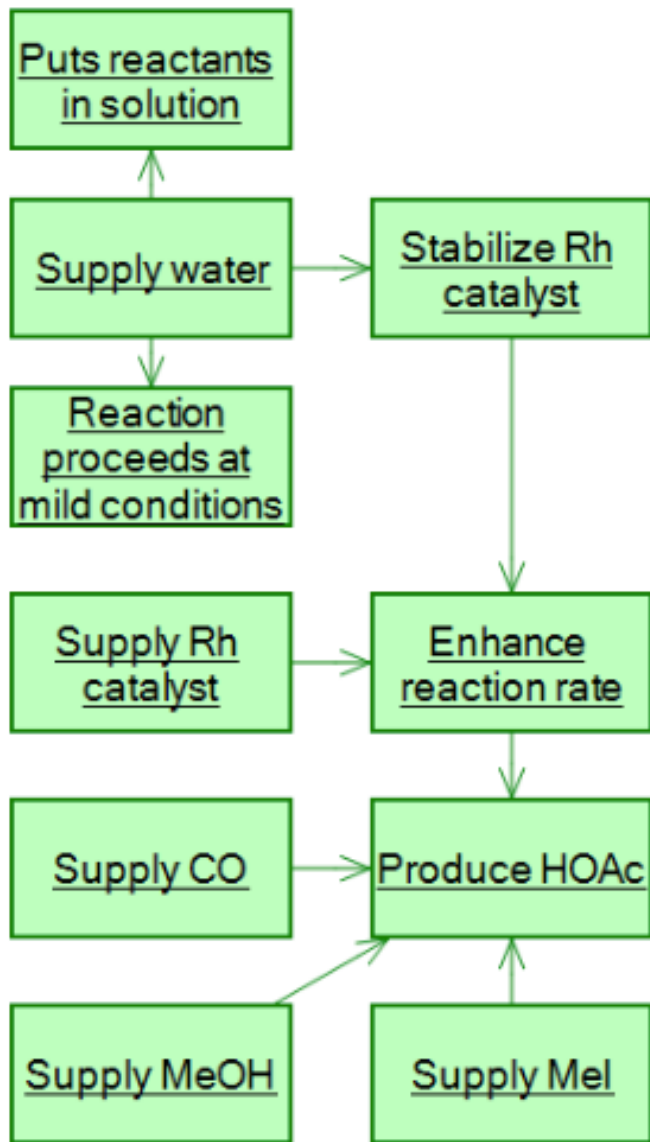
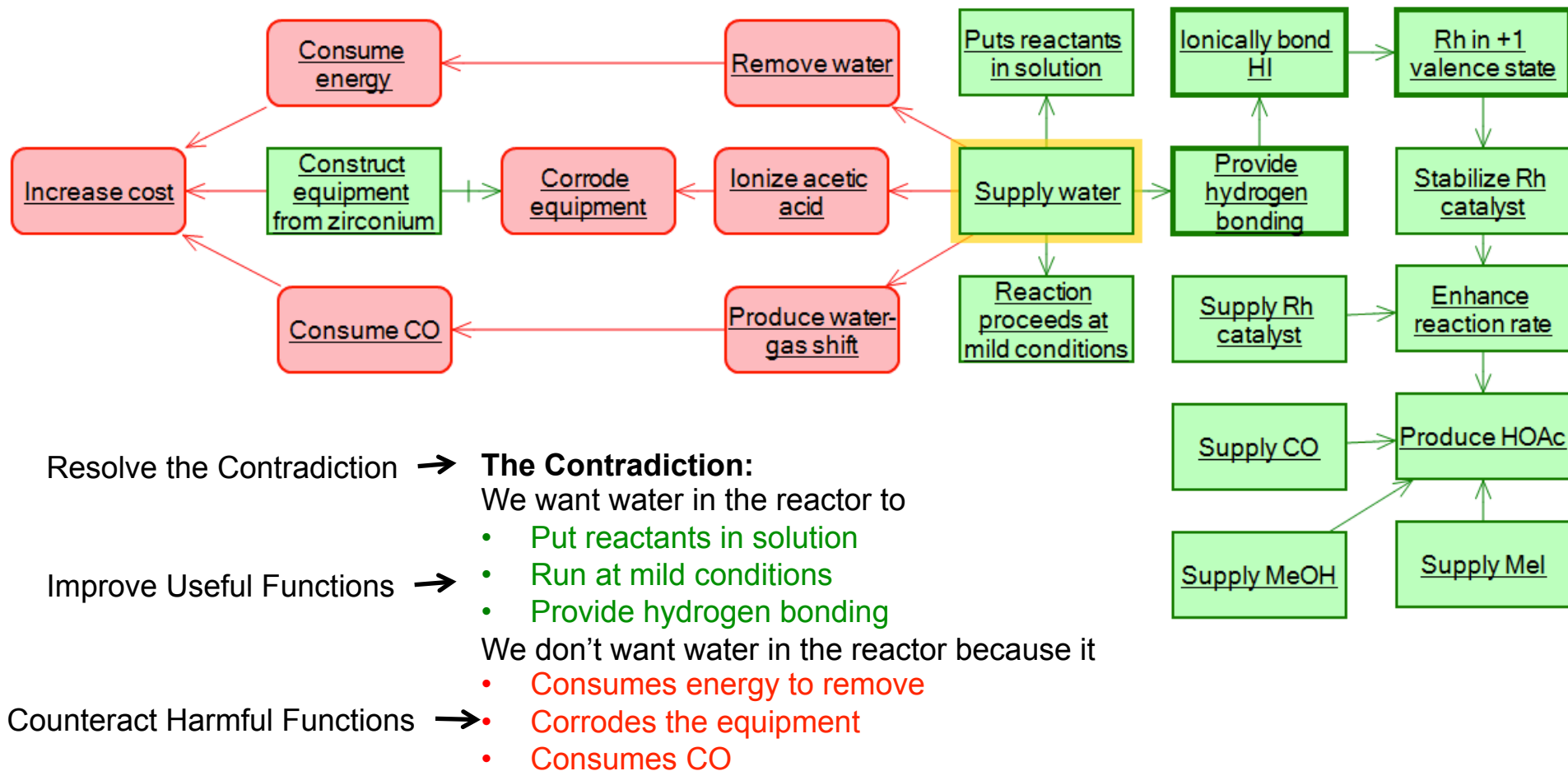# *Refined Process Function Model*
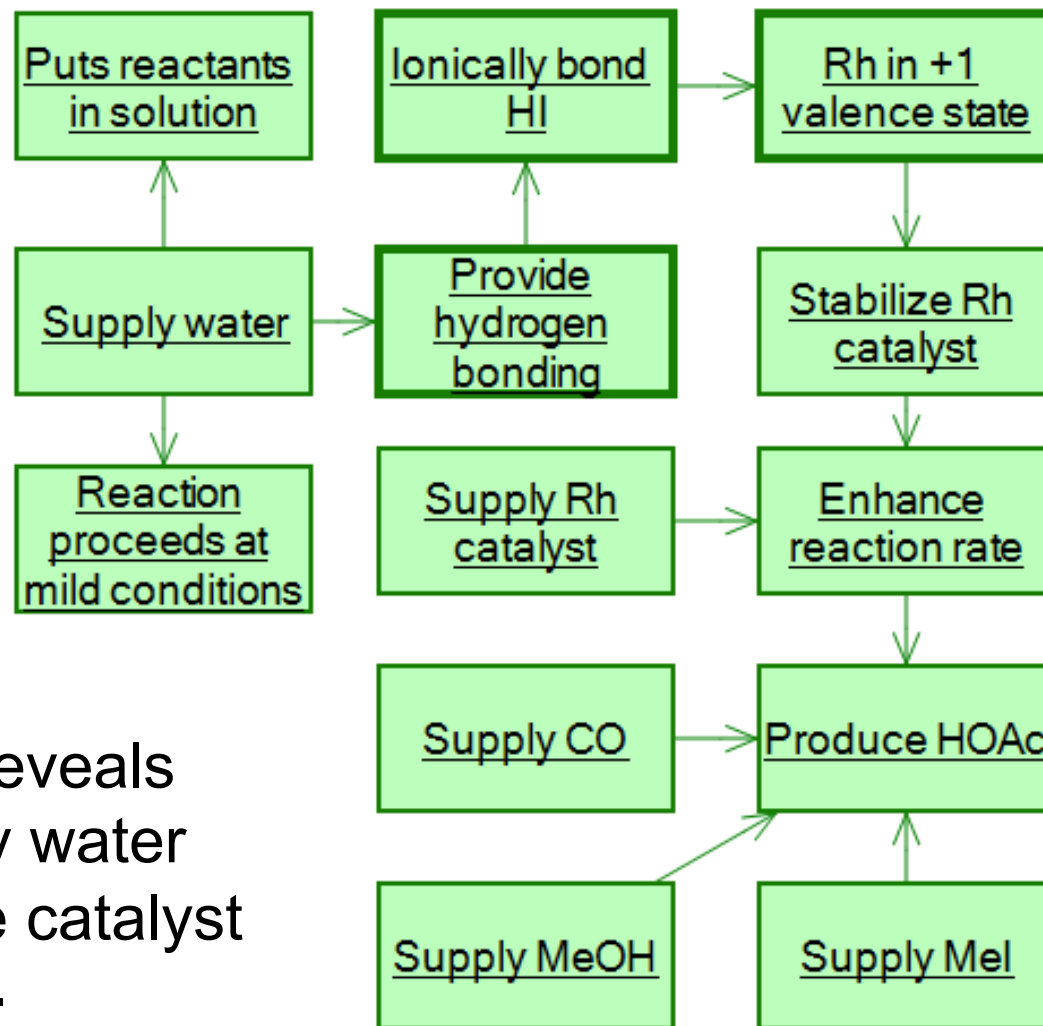


This model reveals how and why water stabilizes the catalyst

# *The Function of Water in the Reaction*



Resolve the Contradiction →

Improve Useful Functions →

Counteract Harmful Functions →

**The Contradiction:**
We want water in the reactor to
- Put reactants in solution
- Run at mild conditions
- Provide hydrogen bonding

We don't want water in the reactor because it
- Consumes energy to remove
- Corrodes the equipment
- Consumes CO

# *TRIZ*

## Resolve a Contradiction by Using Separation Principles

| On Condition | In Structure | In Space | In Time |
|---|---|---|---|
| Find a Condition | Element & Whole | Different Locations | Preliminary Action |
| Dynamism | Use the Culprit | Another Dimension | Synchronization |
| Excessive Action | Partitioning | Nesting | Parallel Processing |
| Partial Action | Integrate | Passing Through | Use Pauses |
| Intensify | Mediator | Take Out a Part | Accelerate |
| Isolate | Use a Model | Localize | Stretch Out |
| Counteract | Feedback | | Post-Process Time |
| Redirect | Controllability | | |

## Improve a Useful Function

| Change Outcome | Change Functioning |
|---|---|
| Intensify | Exclude |
| Disposable | Inversion |
| Universality | Partitioning |
| Specialization | Integrate |
| Dynamism | Mediator |
| Matching | Use a Model |
| Partial Action | Feedback |
| Excessive Action | Controllability |

## Counteract a Harmful Function

| Change Outcome | Change Functioning |
|---|---|
| Eliminate the Cause | Exclude |
| Vaccination | Inversion |
| Isolate | Partitioning |
| Counteract | Integrate |
| Redirect | Mediator |
| Mismatch | Use a Model |
| Restore | Feedback |
| Convert to Benefit | Controllability |

## Mobilize Resources

| Space | Time | Energy/Forces | Substances | Information |
|---|---|---|---|---|
| Vacant Space | Preliminary Action | In the System | System Elements | Properties |
| Another Dimension | Synchronize | Dissipated | Raw Materials | Output Flows |
| Nesting | Parallel Processing | Flows | Waste | Passing Flows |
| Passing Through | Use Pauses | Environmental | Inexpensive | Detection |
| Take Out a Part | Accelerate | Transformed | Transformed | Additives |
| Localize | Stretch Out | | | |
| | Post-process Time | | | |

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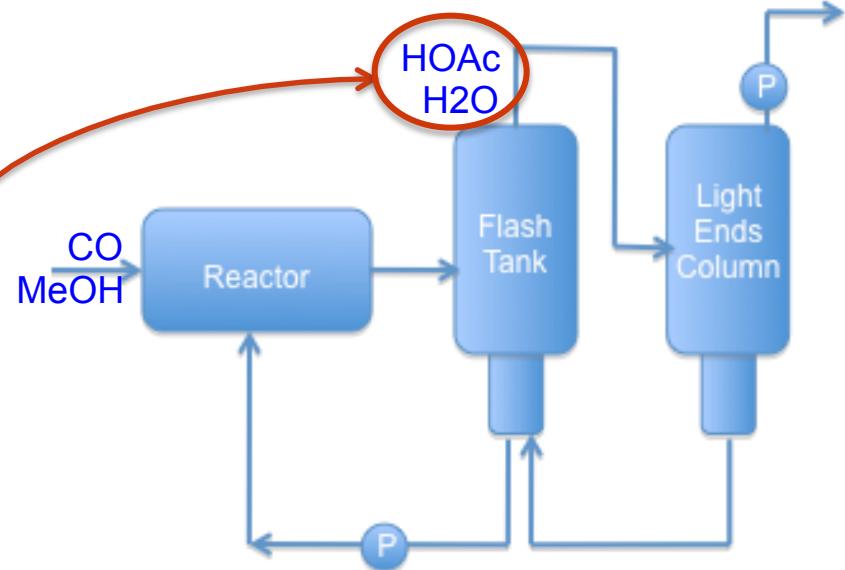phanik@pretiumllc.com

# TRIZ Applied to Acetic Acid

# *Opportunities for Improvement*

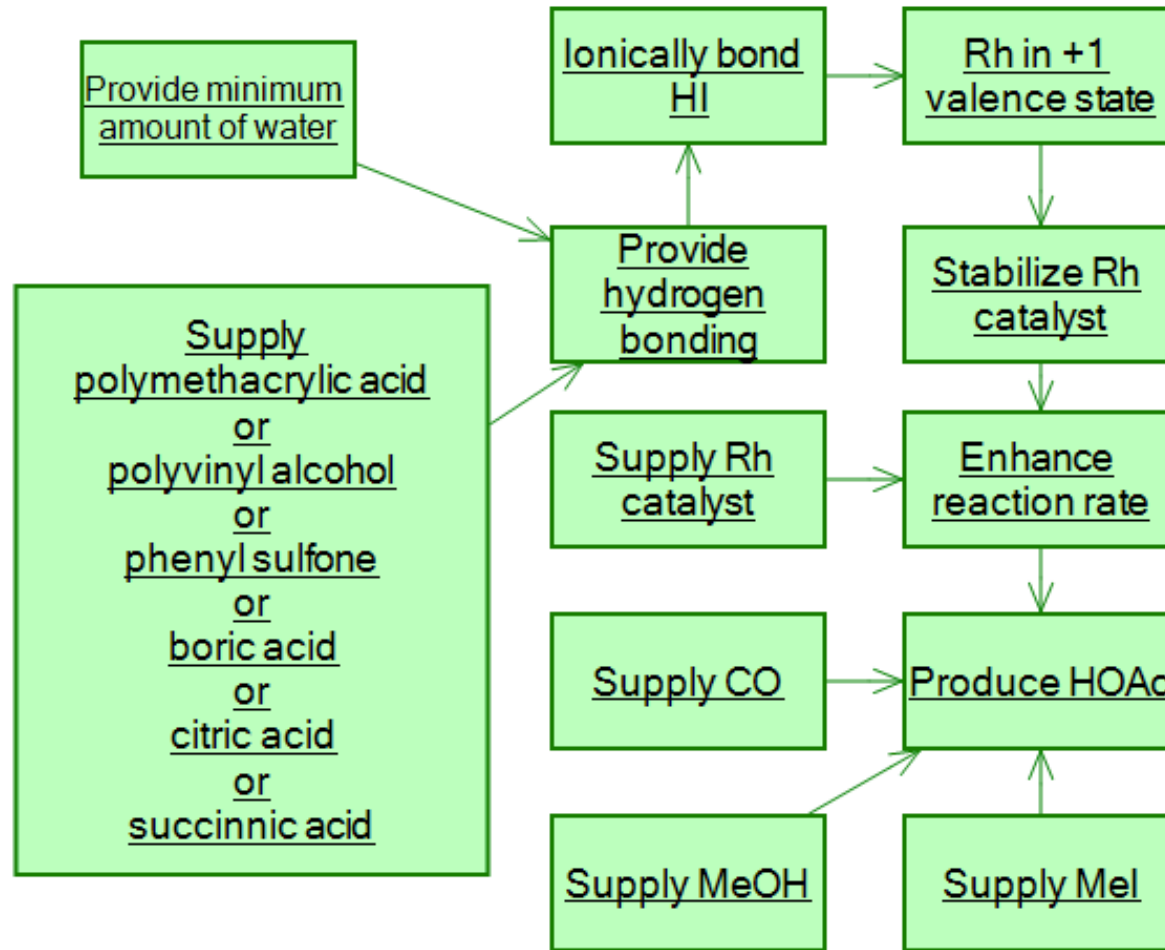Find a Way to Counteract:
"Water must be removed from product".
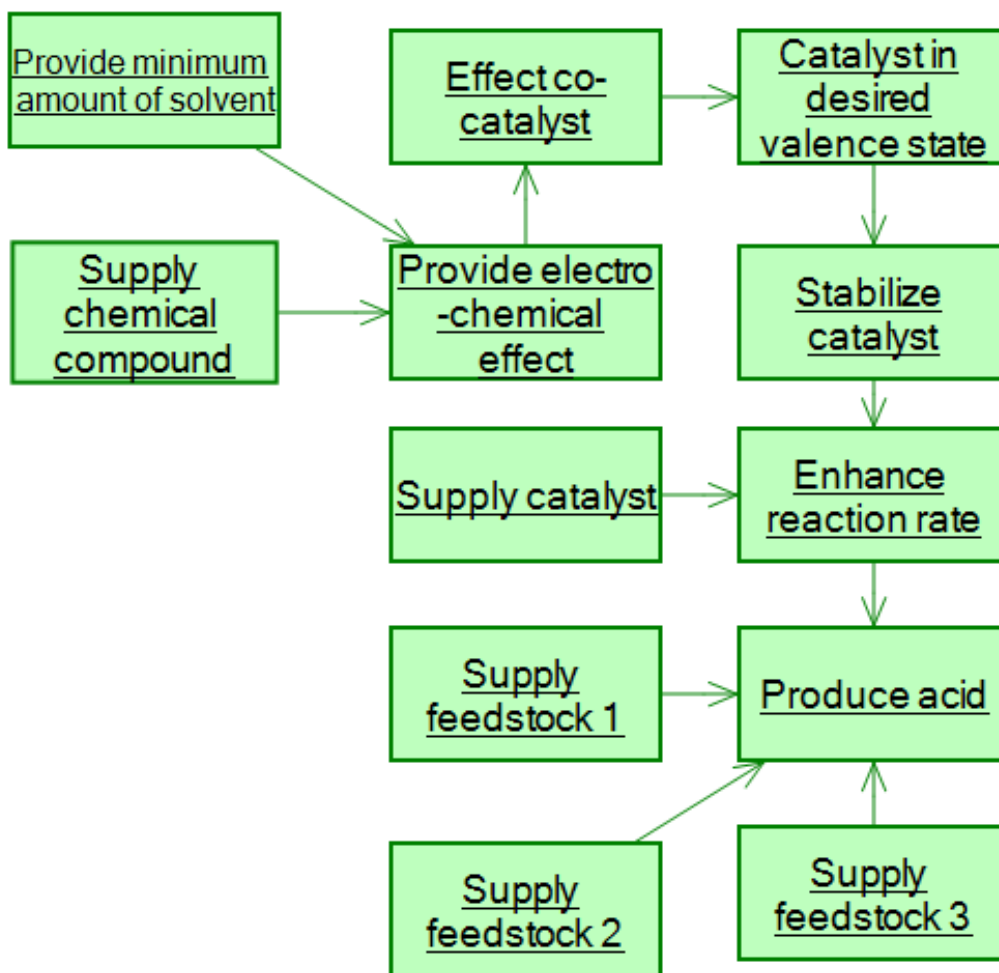
# *Designing the Patent*

# Specific Function Model



The invention as originally conceived by the inventor

# *Pure Function Model*



The pure function model removes specific physicality from the model

# Function Table

| Specific Invention | Patent Base Model | Pure Function Model |
|---|---|---|
| Minimum amt of water | Minimum amt of water | Minimum amt of solvent |
| Supply methacrylic acid, etc | Supply HI solvating agent | Supply chemical compound |
| Ionically bond HI | Ionically bond HI | Effect co-catalyst |
| Provide hydrogen bonding | Provide hydrogen bonding | Electrochem effect |
| Supply Rh catalyst | Supply catalyst | Supply catalyst |
| Supply CO | Supply CO | Supply Feedstock 1 |
| Supply MeOH | Supply alcohol | Supply Feedstock 2 |
| Rh in +1 state | Metal compound stable | Catalyst in desired state |
| Stabilize Rh catalyst | Stabilize catalyst | Stabilize catalyst |
| Enhance rx rate | Enhance rx rate | Enhance rx rate |
| Produce HOAc | Produce Carboxylic acid | Produce acid |
| Supply MeI | Supply alkyl iodide | Supply Feedstock 3 |

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Getting outside of prior art

# *Patent Base Model*
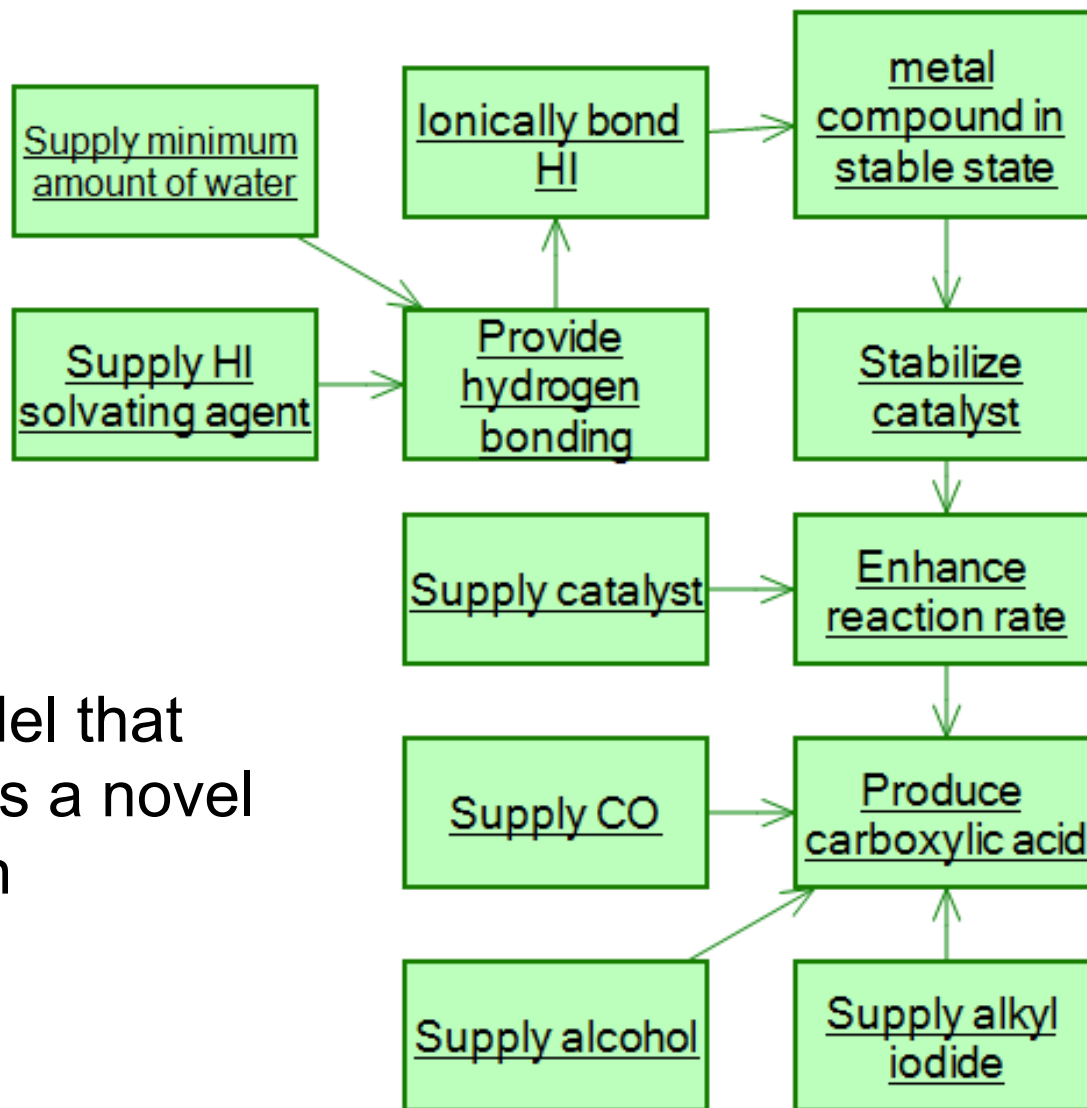


The model that describes a novel invention

# Guided Brainstorming Using TRIZ

| Function | TRIZ Principle | Idea |
|---|---|---|
| Supply HI solvating agent | Specialization | Carboxylic acid |
| | | Polyol |
| | | Sulfone |
| | Matching | Solvating agent w/ high BP |
| | Integrate | Use mixtures |
| Carboxylic acid | Excess action | Polycarboxylic acid |
| | Partial action | Oligomer of carboxylic acid |
| Oligomer of carboxylic acid | Specialization | Polymethacrylic acid |
| Polyol | Partial action | Oligomer containing OH |
| | | Polyol with 2 OH groups |
| | | Co-oligomers containing OH |
| Sulfone | Excess Action | Polymer containing sulfone |
| | | Copolymer containing sulfone |
| | Specialization | Phenyl sulfone |
| Supply catalyst | Integrate | Mixtures of Rh, Ir and/or Pd |
| | Specialize | Rh or Ir or Pd |
| | | Use salts, oxides, organo-comp |

# *Complete Patent Function Model*
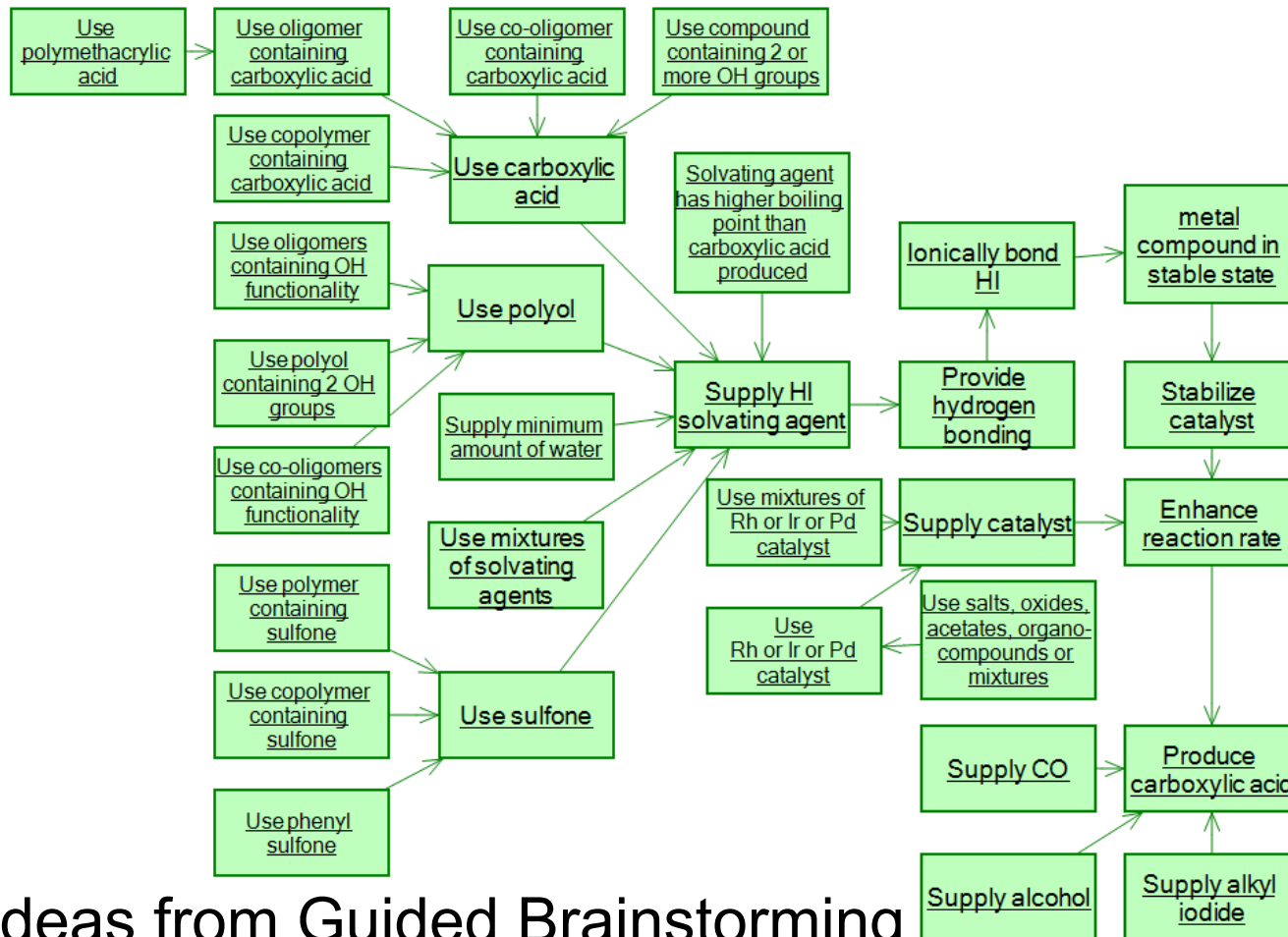


Ideas from Guided Brainstorming are added back into the model

# Foundation Model
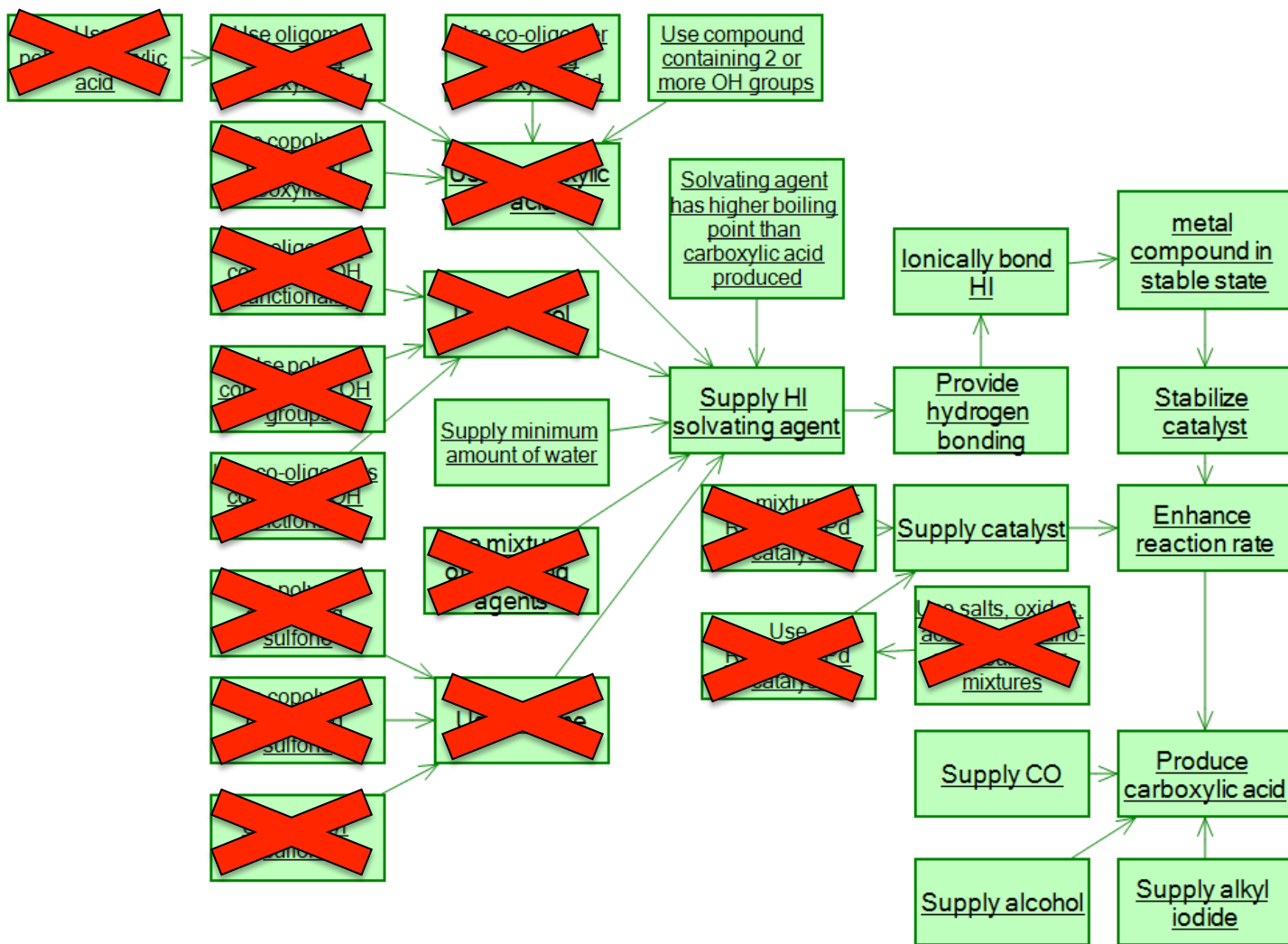
# *Foundation Model*
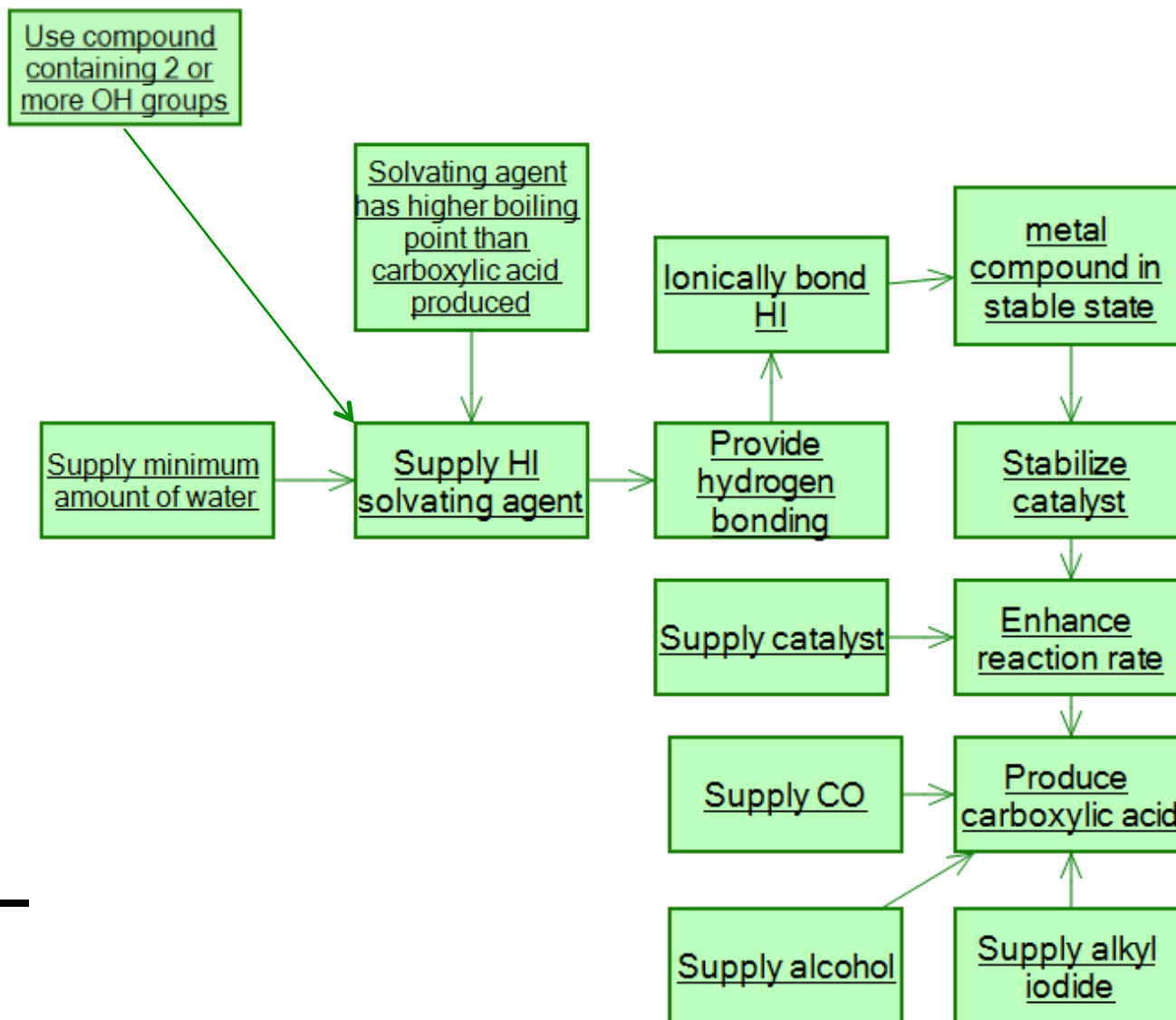
# *Structured Description*

Production of a carboxylic acid by
1. Supplying carbon monoxide
2. Supplying an alkyl halide
3. Supplying an alcohol
4. Enhancing the reaction rate
   A. Supplying a catalyst
   B. Stabilizing the catalyst
      I. Keeping the metal in the catalyst in a stable state
         a. Ionically bonding hydrogen
            i. Providing hydrogen bonding
               ① Supplying an HI solvating agent
                  • Supplying a HI solvating agent with a boiling point higher than water
                  • Supplying a minimum amount of water

# *Structured Description*

① Supplying an HI solvating agent
  A. Use a carboxylic acid
    I. Use compound containing 2 or more OH groups
    II. Use oligomer containing carboxylic acid
    III. Use co-oligomer containing carboxylic acid
    IV. Use polymer containing carboxylic acid
    V. Use copolymer containing carboxylic acid
  B. Use a polyol
    I. ….
    II. ….
    III. ….
  C. Use sulfone
  D. Use mixtures of the above

(54) **COMPOSITIONS FOR CARBOXYLIC ACID PRODUCTION AND METHODS FOR MAKING AND USING SAME**

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(21) Appl. No.: **12/494,098**

(22) Filed: **Jun. 29, 2009**

**Related U.S. Application Data**

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C07C 51/12 (2006.01)
C09K 3/00 (2006.01)
B01J 8/00 (2006.01)

(52) U.S. Cl. ...................... **562/519**; 252/183.11; 422/211

(57) **ABSTRACT**

An alcohol such as methanol is reacted with carbon monoxide in a liquid reaction medium including a catalyst, an alkyl iodide such as methyl iodide, alkyl acetate such as methyl acetate in specified proportions, an additive, and an effective amount of water, where the additive increases an ionic character of the hydrogen iodide bond and the effective amount of water is sufficient to facilitate carboxylic acid release after carbonylation at the catalyst and to reduce anhydride formation. The present reaction system not only provides an acid product at water levels considerable below levels currently used, but also provides unexpected reaction rates and unexpected high catalyst stability.

# Conculsions

- Systematic method produces a solid foundation to broadly define the invention.
- Improved communications between inventor and patent attorney
  - The function models establish a common language for communication
- Write it right the first time
  - Regulations previously proposed under 37CFR would limit the number of continuations to two.
- Provide better information to outside patent counsel with potential to improve quality and reduce costs.
- Brainstorming with TRIZ inventive principles expands the invention and often leads to new inventions.