Nature of Invention: Process design

**Applicant:** NCL

**Inventors:** Prince Yadav

**Chemical Formula:** C5H8O2

**Chemical Name:** Acetylacetone

**Process Title:**

**Process Description:**

1. Give the block diagram for the feasible process (as determined in market analysis report). List all unit operations and process conditions.

**Unit operations and process conditions.**

The **industrial unit operations** involved in the production of **acetylacetone** using the Claisen condensation method, along with the corresponding reactor types for each step:

1. **Mixing (Agitation)**:

- **Purpose**: Ensure uniform distribution of reactants (acetone and butyl acetate) and catalyst (sodium butoxide).

- **Reactor Type**: Stirred tank reactor (STR) or continuous stirred tank reactor (CSTR).

- **Operating Conditions**:

- **Agitation Speed**: Moderate to ensure efficient mixing.

- **Temperature**: Room temperature (around 25°C).

2. **Reaction (Claisen Condensation)**:

- **Purpose**: Formation of the intermediate compound (sodium acetylacetonate).

- **Reactor Type**: Batch reactor or plug flow reactor (PFR).

- **Operating Conditions**:

- **Temperature**: Maintain at 80-85°C for several hours.

- **Pressure**: Atmospheric pressure.

- **Catalyst**: Sodium butoxide (NaOBu).

3. **Cooling and Precipitation**:

- **Purpose**: Allow the product (sodium acetylacetonate) to crystallize.

- **Reactor Type**: Crystallizer (e.g., cooling crystallizer).

- **Operating Conditions**:

- **Cooling Rate**: Gradual cooling to room temperature.

- **Solvent**: Inert solvent (e.g., n-heptane).

4. **Filtration**:

- **Purpose**: Separate the crystals of sodium acetylacetonate from the solvent.

- **Reactor Type**: Filtration unit (e.g., vacuum filter or centrifuge).

- **Operating Conditions**:

- **Filter Medium**: Filter paper or cloth.

- **Pressure**: Gravity filtration.

5. **Acidification**:

- **Purpose**: Convert sodium acetylacetonate to acetylacetone.

- **Reactor Type**: Stirred tank reactor (STR) or continuous stirred tank reactor (CSTR).

- **Operating Conditions**:

- **Acid**: Hydrochloric acid (HCl).

- **Stoichiometry**: 1 mole of sodium acetylacetonate reacts with 1 mole of HCl.

6. **Extraction**:

- **Purpose**: Isolate acetylacetone from the aqueous phase.

- **Reactor Type**: Extraction column (e.g., mixer-settler or packed column).

- **Operating Conditions**:

- **Solvent**: Organic solvent (e.g., dichloromethane).

- **Shaking or Stirring**: To enhance extraction efficiency.

7. **Distillation**:

- **Purpose**: Obtain pure acetylacetone.

- **Reactor Type**: Distillation column (e.g., fractional distillation column).

- **Operating Conditions**:

- **Temperature**: Distill the organic solvent to separate acetylacetone.

- **Pressure**: Atmospheric pressure.

1. Give the material balance for a scaled-up process plant with capacity of 1000 kg/day. (If needed, simplify the calculations by stating assumptions)
2. List the capacity of reactors needed and evaluate the cost. Use Glass lined Carbon steel (GS lined CS) as the material of construction (MOC). Use the pressure according to reaction conditions. You will use only 70% of the total volume. If you design a 1000 L reactor, you can only fill 700 L reaction mixture.

**Capital cost (only for the reactor):**

**example:**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Equipment** | **Design Capacity (L)** | **No. of units** | **Cost/unit ($ for year 2014)** | **Total Cost ($ for year 2014)** |
| Reactor 1  (Jacketed reactor, agitated, Carbon steel, atm. pressure) | 2000 | 1 | 33,500 | 33,500 |
|  |  |  |  |  |

**References:** Provide reference for a research paper or an actual patent.

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**List the contributions of each author:**

* Prince Yadav find out about unit operation and process condition information.
* Authors 2 and 3 found necessary separation steps to achieve desired product purity.

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| Third author Name (if any) |  |  |
| Fourth author Name (if any) |  |  |
| Fifth author Name, Roll No & signature (if any) |  |  |
| Sixth author Name (if any) |  |  |