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# Solid-Liquid Extraction of *Salvia Officinalis* L.: A Simulation Study in Aspen HYSYS

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**ABSTRACT:** Extraction of bioactive compounds from medicinal plants serves as a fundamental step in the production of pharmaceuticals, nutraceuticals, and cosmetics, driven by the increasing preference for natural and sustainable products. This study investigates the application of the Aspen HYSYS simulation tool to model the solid-liquid extraction process for *Salvia Officinalis* L. (Sage), targeting bioactive compounds including rosmarinic acid, carnosic acid, and essential oil. The process employed a solvent system composed of 70% ethanol and 30% water, selected for its effectiveness in dissolving compounds across a range of polarities, particularly phenolic compounds. Simulation results using Aspen HYSYS show that 100 kg of dry biomass yield 4.5 kg of rosmarinic acid, 2.55 kg of carnosic acid, and 0.8 kg of essential oil, all with extraction efficiencies exceeding 85%. The developed model enabled detailed examination of how various parameters affect the extraction of these compounds. Based on the outcomes, this model demonstrates strong potential for scalability and practical use in the solid-liquid extraction of bioactive compounds from medicinal plants.

**KEYWORDS:** *Salvia Officinalis* L., Solid-liquid extraction, Aspen HYSYS simulation, essential oil

## I. INTRODUCTION

Medicinal plants serve as important sources of bioactive compounds with significant therapeutic potential. Among these, *Salvia Officinalis* L. stands out. Researchers often focus on this species due to its high concentration of diverse phytochemicals and recognized pharmacological properties (Perry et al., 2003; Hamidpour et al., 2014). Native to the Mediterranean region, *Salvia Officinalis* L. contains several secondary metabolites that contribute to its antioxidant, antimicrobial, and anti-inflammatory activities (Lu & Foo, 2001; Mimica-Dukić et al., 2003). Key bioactive constituents in *S. officinalis* include rosmarinic acid, known for its antioxidant and anti-inflammatory actions (Petersen & Simmonds, 2003). Carnosic acid, a diterpene, exhibits antimicrobial and neuroprotective properties (Birtić et al., 2015). Its essential oils feature compounds like thujone, camphor, and 1,8-cineole, which are linked to antimicrobial and aromatic effects (Bozin et al., 2007). With growing demand for natural plant extracts, researchers now pay considerable attention to selecting and refining extraction techniques. Within this context, solid-liquid extraction emerges as the primary method for isolating bioactive compounds from plant materials, offering effective recovery and wide applicability in phytochemical studies (Rostagno & Prado, 2013).

Extracting bioactive compounds from plants comes with a set of real hurdles. Compound polarity, for one, is all over the map. The rosmarinic acid compound is very polar but essential oil, though, sits on the non-polar end. This difference calls for a solvent that can handle a broad range, as highlighted by Durling et al. (2007). Temperature sensitivity also complicates extraction. Raising the temperature definitely bumps up mass transfer rates, but compounds like phenolic acids and diterpenoids don't tolerate heat well (Rostagno & Prado, 2013). Mass transfer itself is slowed by the tangled, intricate structure of plant materials (Cassel & Vargas, 2006). From the process side, cost and environmental concerns weigh heavily. Solvent expenses stack up fast, and so does the need to minimize environmental impact (Chemat et al., 2017).

## II. LITERATURE SURVEY

Researchers have explored a range of methods for extracting bioactive compounds from *Salvia Officinalis L.*, including both traditional techniques like maceration and Soxhlet extraction, and modern methods such as ultrasound-assisted and supercritical fluid extraction (Rostagno & Prado, 2013; Chemat et al., 2012). Among these, solid-liquid extraction (SLE) stands out as a preferred technique for *Salvia officinalis L.* because it is straightforward, scales up easily, and uses food-grade solvents (Durling et al., 2007). Findings consistently show that using a mix of ethanol and water as solvents achieves high extraction efficiency for phenolic compounds like rosmarinic acid. This effectiveness originates from the polarity of the solvents, which enhances both solubility and diffusivity (Michielin et al., 2011; Teixeira et al., 2013). Beyond phenolics, studies also demonstrate that this solvent combination works well for extracting moderately non-polar compounds such as diterpenes like carnosic acid and essential oils, since ethanol-water blends can boost their solubility (Birtić et al., 2015; Bozin et al., 2007). Researchers have been focusing on optimizing extraction conditions such as temperature, solvent composition, and solvent ratio to increase product yields while reducing energy consumption and avoiding the breakdown of thermolabile compounds (Dorman et al., 2003; Rostagno & Prado, 2013). Most studies so far rely on experimental approaches, which can take a lot of time. Simulation tools like Aspen HYSYS, often used in chemical and pharmaceutical industries for separation processes, have not seen much use in natural product extraction (Ghasem & Redhouane, 2018; Jones & Ogden, 2016). Thermodynamic simulation tools, for instance, the NRTL equation, allow researchers to predict phase equilibrium within these systems (Renon & Prausnitz, 1968).

## III. METHODOLOGY

The biomass composition of *Salvia officinalis* was determined using literature data concerning the dried leaves of the plant (Lu & Foo, 2001; Perry et al., 2003). According to these sources, the typical composition includes 5% rosmarinic acid, 3% carnosic acid, 1% essential oils, and 91% inert matter. These concentrations reflect the common distribution of phytochemicals in plant materials and are essential for accurate extraction modeling.

In this study it is selected a 70:30 ethanol to water ratio for its solvent mixture due to two main factors. Ethanol dissolves non-polar compounds well, while water enhances the extraction of polar compounds. This combination improves overall extraction efficiency. Additionally, ethanol offers a sustainable and safe option as it is both renewable and approved for use in food and pharmaceutical production. To illustrate the extraction process, it is developed a detailed process flow diagram (PFD) using Aspen HYSYS (see Figure 1). The diagram covers three main stages: first, the mixer combines the feed with the solvent; next, the extractor simulates the mass transfer between the feed and the solvent; finally, the separator recovers the extracted compounds and leaves behind the spent feed.

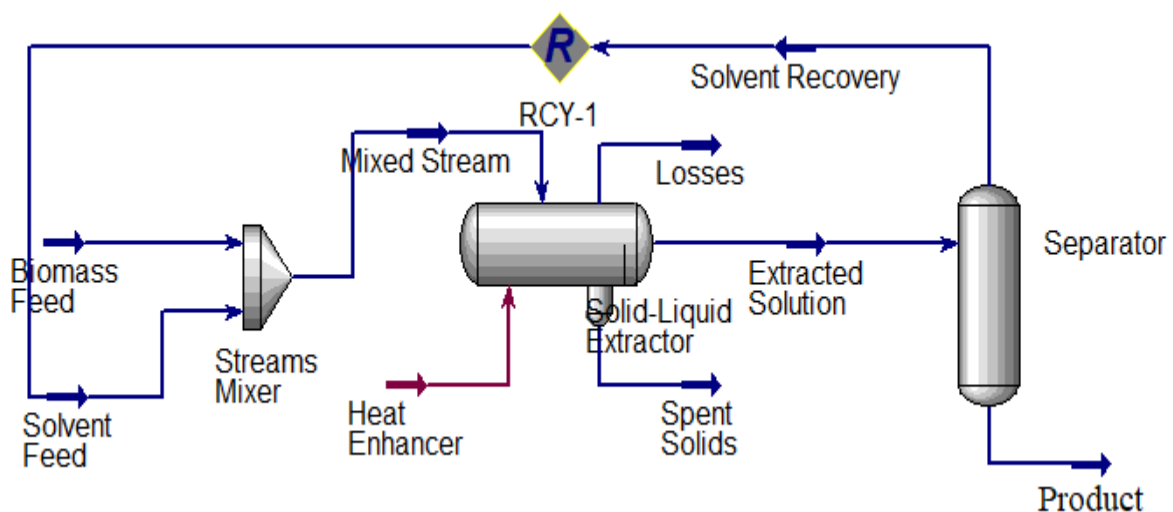


Fig.1 *Salvia Officinalis L.* extraction simulation process diagram

The Non-Random Two-Liquid (NRTL) thermodynamic model predicts phase equilibria in systems where non-ideal behaviors are pronounced. This approach is particularly suited for mixtures involving polar solvents or organic compounds, as it supports accurate estimations of molecular interactions and activity coefficients (Renon & Prausnitz, 1968). Its relevance becomes even more evident in ethanol-water mixtures containing bioactive compounds, since these systems demonstrate significant non-ideality. Simulations used operating parameters that reflect typical industrial-scale solid-liquid extraction (SLE) conditions. Biomass entered the system at a dry feed rate of 100 kg/h. The solvent, a blend of ethanol and water at a 70:30 volume ratio, was introduced at a steady rate of 500 kg/h. Temperature and pressure were held constant at 40 °C and 1 atm throughout the process. Selecting a 5:1 (w/w) solvent-to-biomass ratio was based on established literature, as this configuration optimizes extraction efficiency in industrial SLE applications (Teixeira et al., 2013). Extraction efficiencies for the target compounds were determined from literature and applied directly in the simulation model. Rosmarinic acid was set at 90%, reflecting its high solubility in polar solvents, as reported by Rostagno and Prado (2013). Carnosic acid had an extraction efficiency of 85%, given its moderate lipophilicity. Essential oils were assigned an extraction efficiency of 80%, aligned with their partial solubility in ethanol-based solvents (Michielin et al., 2011). These efficiency values match experimental data from *Salvia Officinalis* L. extraction performed under comparable conditions.

#### IV. EXPERIMENTAL RESULTS

The simulation results confirm that the selected solvent system efficiently extracts the target compounds (Table 1). Rosmarinic acid showed the highest extraction efficiency due to its polarity, while essential oils were effectively extracted due to ethanol's solubilizing capability (Durling et al., 2007; Bozin et al., 2007). The obtained yields are consistent with experimental data reported in the literature, which typically range between 80–95% for phenolic compounds (Teixeira et al., 2013).

Table.1 Essential oils extraction efficiency

| Compound        | Initial Mass (kg) | Extracted Mass (kg) | Efficiency (%) |
|-----------------|-------------------|---------------------|----------------|
| Rosmarinic acid | 5                 | 4.5                 | 90             |
| Carnosic acid   | 3                 | 2.55                | 85             |
| Essential oils  | 1                 | 0.8                 | 80             |

The composition of the solvent plays a crucial role in determining the efficiency of the extraction process. A mixture of 70% ethanol and 30% water offers an optimal balance between polarity and solubility, which aligns with findings from previous research (Michielin et al., 2011). When ethanol concentration is lower, the extraction of non-polar compounds decreases, while a higher ethanol concentration reduces the solubility of polar compounds (Pavia et al., 2008) (Table 2).

Table2. Effect of solvent composition in yield

| Ethanol-Water Ratio (w/w) | Yield of Rosmarinic Acid (kg) | Yield of Carnosic Acid (kg) | Yield of Essential Oils (kg) | Observations   |
|---------------------------|-------------------------------|-----------------------------|------------------------------|--|
| 50:50                     | 3.8                           | 2.2                         | 0.6                          | Lower yield due to reduced ethanol concentration for non-polar compounds.              |
| 60:40                     | 4.2                           | 2.4                         | 0.7                          | Improved extraction due to better solubility balance for polar and non-polar compounds |
| 70:30                     | 4.5                           | 2.55                        | 0.8                          | Optimal solvent ratio achieving maximum yield for all target compounds                 |
| 80:20                     | 4.0                           | 2.3                         | 0.75                         | Reduced efficiency for polar compounds due to excess ethanol                           |

Temperature plays a key role in both solubility and diffusion rates. Maintaining the temperature at 40 °C supports efficient mass transfer with minimal compound degradation. When the temperature rises above 55 °C, significant degradation of bioactive compounds occurs, which negatively impacts extraction outcomes (Table 3).

Table3. Effect of Temperature on Extraction Efficiency

| Temperature (°C) | Extraction Efficiency of Rosmarinic Acid (%) | Extraction Efficiency of Carnosic Acid (%) | Extraction Efficiency of Essential Oils (%) | Observations  |
|------------------|--|--|---|---|
| 25               | 80   | 75   | 70  | Lower efficiency due to reduced solubility and slower mass transfer   |
| 40               | 90   | 85   | 80  | Optimal efficiency for all compounds with minimal thermal degradation |
| 55               | 84   | 78   | 74  | Slight decline due to nearing thermal sensitivity thresholds          |
| 70               | 72   | 66   | 60  | Significant decline due to thermal degradation of bioactive compounds |

The ratio of solvent to solid also influences extraction efficiency. A 5:1 ratio achieves optimal results, while increasing the ratio further offers no substantial gains (Table 4).

Table4. Effect of Solvent-to-Solid Ratio on Yield

| Solvent-to-Solid Ratio (w/w) | Yield of Rosmarinic Acid (kg) | Yield of Carnosic Acid (kg) | Yield of Essential Oils (kg) | Observations   |
|------------------------------|-------------------------------|-----------------------------|------------------------------|--|
| 3:1                          | 3.8                           | 2.1                         | 0.6                          | Insufficient solvent volume leads to incomplete extraction                         |
| 4:1                          | 4.2                           | 2.4                         | 0.7                          | Improved yield but slightly lower than optimal due to limited solvent saturation   |
| 5:1                          | 4.5                           | 2.55                        | 0.8                          | Optimal yield with adequate solvent for mass transfer and solubilization           |
| 6:1                          | 4.5                           | 2.55                        | 0.8                          | No significant improvement despite higher solvent volume, leading to inefficiency. |

## V. CONCLUSION

The study demonstrates that Aspen HYSYS effectively simulates the solid-liquid extraction process for *Salvia officinalis*, offering comprehensive insights into mass transfer, equilibrium, and overall efficiency. The combination of 70% ethanol and 30% water provides an optimal balance of polarity, facilitating the extraction of both hydrophilic and moderately lipophilic bioactive compounds. Results confirm that key process variables such as temperature, solvent composition, and the solvent-to-solid ratio, significantly influence extraction efficiency. Furthermore, with the help of simulation tools like Aspen HYSYS, various operating conditions can be quickly analyzed using simulation techniques, which is helpful in saving time and resources during the development phase. This is particularly important in green extraction technologies, as optimization is critical to meet environmental and regulatory requirements.

In future, this study can be extended to validate the simulation results using experimental methods to further validate the accuracy and reliability of this simulation-based approach. Moreover, downstream processes like distillation,

purification, and separation can also be incorporated to develop a comprehensive process flow to recover high-purity products from natural bioactive compounds. Advanced simulation techniques like kinetic modeling and LCA can also help in developing a more accurate picture of the process from a green perspective. Overall, this simulation-based approach combined with experimental techniques is a significant move towards developing natural bioactive compounds in industries.

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