Simulation Of Coffee Stain Effects Using ANSYS Fluent

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Abstract. The following project takes an investigative look in the commonly observed coffee stain effect in fluid dynamics that explains the arrangement and alignment of particles and droplets when subjected to an evaporative flux. The primary objective of the paper deals with the methodology and results obtained by the simulation of the effect in ANSYS fluent and the parameters used to produce the effect. The latter part of the project studies the relation between surface energies and contact angles for droplets and seeks to develop a relationship between both. The coffee stain effect has been further replicated using Surface Evolver, Energy 2D and the FEA Multiphysics Toolbox from MATLAB. Coffee stain simulations are a greater way of interpreting a widely known phenomenon that have captivated the interests of researchers and the following report intends to understand such dynamics and replicate them in software environments.

1. INTRODUCTION

The coffee-ring effect is a phenomenon of wide interest to the academic circles of fluid mechanics and heat transfer by being studied and replicated on software environments. This project will aim at understanding the phenomenon of coffee stains on surfaces.

The coffee-ring effect is a common phenomenon observed in various experiments including those involving liquids, colloidal suspensions, aerosols and binary mixtures. The project aims to simulate an environment for a binary phase mixture and study the effects that contribute to the effect while working on multiple softwares. ANSYS FLUENT is the primary software on which the model was created.

Further studies were also conducted using Surface Evolver, Energy 2D, and the QuickerSim ToolBox from MATLAB. The phenomena of the formation of coffee stains is directly related to the drying of a region of a drop which is mainly suppressed to prevent the further spread of particles and to avoid the expansion of the ring.

The project focuses on studying and simulating these effects mainly in the ANSYS fluent environment and also other lesser known additional softwares.

Previous studies conducted on the spread and dynamics of droplets reveals forces that contribute to the expansion of the particles as well as how the forces can be manipulated to suppress and concentrate the spread to a single point rather than occupying a greater circumference. The coffee-ring effect has been observed in various experiments including those involving liquids, colloidal suspensions, aerosols and binary mixtures [1].

The phenomena of the formation of coffee stains is directly related to the drying of a region of a drop that contains particles which causes particles to accumulate at the contact line. Initial studies conducted by Langmuir and Deegan to describe the shape of a spherical drop suspended in air were
instrumental in devising a new subset of fluid flow effects which asserts the shape to be the cause of an outward radial flow of the drops facilitated by evaporation [2].

Literature data suggests that in order to replenish the loss of solvent particles at the contoured contact line, the liquid flows in a radial manner. The manner in which the particles in the drop are transported and scattered is determined by the flow field in the drop and the evaporation profile.

However the laminar radial flow is subject to change as the liquid composition varies with the temperature profile. Thermal or solute rich Marangoni effects have been studied as they can contribute to a turbulent flow in a binary solvent or a reverse flow from surfactant concentration gradients. Instead of evaporating from the liquid Vapour interphase, the absorption by the substrate has also known to modify the deposition of the particles in order to create a more constant shaped coating [2].

For simple liquids characterized by a laminar radial flow, the transport of particles suspended in a evaporating drop depends solely on the evaporative flux. To describe the particle accumulation at the contact line, it is necessary to specify that the evaporative flux again is a function of the solvent diffusion in the gas phase, and the shape of the liquid-Vapour interface. Mathematically, the coffee stain effect has been surmised using finite element methods for erratic evaporating fluids. Relations between diffusive concentration fields and electrostatic potential fields allege that the phenomena can be understood as a tip-shape effect [3].

A second approach to understand the effect has been through Monte Carlo simulations that designs particles on the discrete lattice and calculates the estimated trajectories of the particles in motion. Previous attempts to translate the effect using Monte Carlo equations have either not considered the velocity components in the vertical dimensions and merely relies on the radial motions [4].

Further studies have modeled the coffee stain growth in two dimensions using Poisson-like process of random particle deposition which again only takes into account the vicinity of the contact line and has not considered droplet evaporation and inward flow dynamics. The Monte Carlo approach has been used with a biased random walk (BRW) to understand the changes that occur from the coffee-ring deposition to a uniform circular shape that shows a full 3D structure of the coffee ring along with a profile of thickness.

The evolution of the ring shape and dimensions is observed during the entire time period of the droplet drying. The lattice structure usually takes the shape of a pinned sessile droplet with a spherical cap and a pre-defined initial contact angle value and an apex height. The domain of the droplet boundary continuously reduces in the direction of evaporation while the shape remains a spherical cap as the contact angle value drops continuously as time goes on [1].

While methods to suppress the coffee stain involve altering of the parameters of the flow, other methods such as electrowetting methods used for suppressing the coffee stain growth which exert interactive forces directly to the contact line of the sessile drops.

The Brownian rendering of the particle ordering can be represented as a comparison of time scales: on the one hand, the Einstein-relation timescale $\tau = d^2/D$, where $d$ is the particle diameter, and $D$ the particle diffusivity; on the other hand, the hydrodynamic timescale $\tau = L/u$, where $L$ is the average distance between nearby particles (a function of particle concentration). When both coincide the critical velocity becomes $u \sim LD/d^2$ [5].

When a sessile droplet rests on a horizontal surface, it causes the water droplets to gradually evaporate and leave a ring-shaped stain after drying, which is called the coffee-ring effect. This is highly undesired in major applications such as inkjet printing and protein microarrays that require a streamlined coating of solid contents after drying. Other efforts to remove the coffee-ring effect
include capillary force methods, Marangoni effects, and addition of surfactants. Research has also shown that when suspended in ellipsoid shapes, particles in the coffee stain effect show a uniform spread as they cling to and float at the air-water interface [6].

Because the air-water inter-face surrounding the floating non-spherical particles is highly hindered, it would cause a significantly enhanced particle-particle attraction producing a single layer of resistance that prevents the particles from moving towards the edge. A small number of ellipsoids is sufficient to destroy the coffee-ring effect.

The project in its crux will shed some light on the various methods through a simulation while comparing the efficiencies of the various discussed methods of suppressing the spread while also experimenting with inward flow dynamics. Studies with suspended particles will focus on their tendency to kinetically accumulate at the air-liquid interface and deposit uniformly.

As the interface shrinkage rate reaches a high level the particle average diffusion rate, particles in vertical evaporation flow will be captured by the descending surface, producing surface particle jam and forming viscous quasi-solid layer, which dramatically prevents the trapped particles from being transported to drop edge and results in uniform deposition [7].

If the droplet dries rapid enough, particles tends to accumulate at the air-liquid interface rather than at the drop edge and directly deposit in the interior. In such scenarios, introducing flows that counteract the evaporation-driven ones can minimize the deposition of solutes at the contact line. Other strategies include the addition of force fields, simply preventing them from being carried along with the evaporation-driven flows [2].

In this case, the coffee-ring effect is suppressed regardless of the presence of the pinning of the contact line and the resulting flows towards the contact line using photosensitive cationic surfactants, which induced stickiness of anionic nanoparticles. Ellipsoidal particles fall under the bracket of shape-dependent capillary attractions to form homogeneous disc-like residues. This method is suitable for hydrophilic surfaces. Unfortunately, it is successful only when large amounts of ellipsoidal particles are present in the droplet. Acoustic vibrations are also a viable method to suppress the stains.

2. METHODOLOGY

The project involves an assessment of the processes that contribute to coffee stains and modeling the same in a powerful software like ANSYS Fluent. It will further assess factors that affect the process by applying various conditional parameters to the drop. For comparative studies, the critical flux model, k-flow method and boiling phase model have been used in the ANSYS Fluent examples.

The project will initially focus on understanding the effects from literature which will be replicated onto a computer environment. Factors that affect it can possibly be studies using analytic tools like MATLAB. In the very same software, models have been incorporated using the Lagrangian method, critical heat flux model and the Eulerian model with standard temperature and pressure setups.

The ANSYS Fluent environment contains various empirical models that have been employed in replicating the effects to their maximum congruency.

In terms of the effects on the shape and spread of the drop, the Surface Evolver and Flowsquare environments have been used that use similar models and can be programmed to include specific cases for different contact angles. Among both, the Eulerian model, mixing and non-mixing cases has been used and shown.

Parameters such as mixing coefficients, temperature, pressure, initial concentrations and others have been taken into account for certain models.[8]
The ANSYS Workbench environment is well equipped with the necessary tools and models to study the coffee stain effect. In order to design the drop, it is represented as a flat semicircle for initial studies and is designed in the Design Modeler section with an initial mesh element size of 0.6 units. The design has been specified to hold separate contours for the lower base of the drop and the outer semicircle using named selections.

The accuracy of the models were linked to a required meshing size which was kept to a modest level to ensure proper results. A higher mesh count with a smaller unit size leads to greater use of computing spaces but produces more coherent results. Choosing an appropriate mesh size makes the difference in balancing the time and clarity of the results produced.

The Mesh Design is then studied by applying a standard user defined function model for the velocity profile. The first output model assumes an inlet velocity from the base and outward pressure boundary condition on the semi-circular shape. The resultant shape shows velocity contours spreading outward representing an air and water mixture dispersing and settling with time.

Separate properties for the system dynamics were set such as velocity, pressure, temperature and separation using named selections. In this case the named selections allow for an easier demarcation of the boundaries and conditions imposed on the drop.

3. RESULTS

The following simulation runs were conducted by using a circular quadrant as the mesh for the geometry. The base of the drop was assumed to be a wall for the boundary conditions while a output pressure boundary condition was placed on the outer curve. The axis was modelled to have an asymmetric case such that the simulation would be identical to that of the other side. Temperatures were set to mimic boiling conditions (373 K) with outward pressures varying by small amounts from the pressure set inside the boundaries.

The aim for the current model was to simulate a Marangoni flow for the water and air fractions in the drop which would ultimately suppress the water and to study the velocity vectors.

![Figure 1 Water volume fraction model. (Boundary conditions: Base is set to be a wall, a pressure outlet for the curved boundary and asymmetric for the axis)](image1)

![Figure 2 Water vapor air model. (Boundary conditions: Base is set to be a wall, a pressure outlet for the curved boundary and asymmetric for the axis)](image2)

To illustrate the differences in the occupation of water by air, the Figure 1 and Figure 2 show how the air component first initiates contact by creating a curved area that is demarcated from the water component with a mid-pressure level area represented by yellow in the figure below.

Pressure studies consistently show that low pressures dominate the outer curved contours while higher pressures are found at the site of interaction where the species are interchanged and successive change in volume fraction of the components takes place. These effects have been validated further from tabular analysis of surface conditions in simulations from the literature[3].
To implement this, a DEFINE INIT condition was placed which specified that the volume fraction for water be set at 1.0 around the centroid and 0.0 elsewhere, occupying fifty percent of the mesh area. Similarly, for air, the function was used to set its fraction at 0.0 near the centroid and 1.0 around the outer contour. The ANSYS FLUENT Window initialized the pressure to atmospheric conditions with an implicit body force selection and patched air to occupy fifty percent of the mesh area.

In order to induce a Marangoni type flow, a DEFINE ADJUST function was used which reduced the cell fraction value by 0.01 wherever the water volume fraction was found to be between 0.0 and 1.0. The simulation results showed that as time progresses, the quadrant interphase slowly suppresses the water region moving towards the center in the action of swirling eddy velocity currents reminiscent of Marangoni stress vectors. The swirling eddies are at their maximum action between the interphase and air region and grow weaker and weaker once a certain fraction of water has been suppressed.

These swirling motions and effects can be seen partially in the Figure 3, below where the change in volume fractions leading towards the center can be seen for air. These shapes are characteristic of the von Karman vortex commonly found in candle wicks and interestingly in droplet shape studies. The figure shows the intermediate change in volume fraction that occurs by being facilitated by forces acting towards the center.

![Figure 3 Suppression contours. (Boundary conditions:- Base is set to be a wall, a pressure outlet for the curved boundary and asymmetric for the axis)](image)

**Velocity Profiles**

The following images show the velocity profile schemes where a transition in the velocities to a swirling type arrangement was observed as time proceeded. All schemes employed a boundary condition where the base was set to be a wall, a pressure outlet for the curved boundary and symmetric for the axis. Mass fractions were set equally for both water and air (0.5 and 0.5).

The images show the waning concentration of the bottom component which allows for a rising concentration of the outward component. Velocities swirl in a recurring circular motion as shown in Figure 2 to drive out the components. Figure 4 and Figure 5 below shows a case where the water phase was initialized to occupy a much larger volume than the air phase. On taking a further look at the figures, we can see that as we move from the center of the quadrant to the phase separation zones (represented by light yellow to yellow blue), the effect of the velocities for the water phase gradually increase leading to a special zone where they interact with the velocities of the air phase. Some velocities at the edges of the contours have water components as well indicating that it is being pushed out and drawn away. The gradual reduction in the volume fraction of the water component can be seen in Figure 2, where the separation zone lowers and continues to show vectors that cross into each other.
The figures discussed in this section all purport that the use of the multiphase model with well set parameters produce the swirling and recurring motions of the components that make it a god fit for studying the Marangoni flow vectors. The water to vapor ratio is taken up by water vapor which slowly dominates the entire boundary till the mass transfer effects roll away the water components and the droplet is ultimately suppressed.

A further and more definite look at the Figure 6 and Figure 7 show a good evidence for the presence of circular mass transfer zones which are well co relational to the Marangoni effect. The figures also show regions where the mass transfer becomes inactive with time and the gradual outward movement of the mixture phase component which indicates that in a boiling model, mixture components tend to ‘escape’ the system towards the end leaving a suppressed droplet. In order to validate these models, the simulation parameters were placed in unsteady state models as set by the system and confirmed for accuracies based on convergence of resultant equations.

If the models were to diverge, the results were discarded due to the lack of proper phase demarcations.
Figure 8 provides a more compelling case for the dynamic nature of the dual phases that interact with each other to produce a counteractive swirling motion that ultimately focuses towards the centre. These findings are closely related to the phenomenon that have been observed from previous studies, especially for Eulerian and heat exchanger enabled k equation simulations [9].

Surface Evolver Design-General Model
A three dimensional view of the droplet evaporation scheme has been created in surface evolver to study the effects of various energies and contact angles on the droplet surface. The boundary conditions for all surface evolver cases have been set to apply a wall condition to the base with an outward velocity condition to the curved outer boundary.

Figure 10 shows the final mesh scheme for the sessile drop at its angle with predetermined pressure and temperature values. On comparing the resultant surface energies with angles it can be inferred that the values tend to reach a certain value with higher angles till a constant value is reached.
These figures show the final orientation of the drops when moving from a hydrophobic to a hydrophilic side. These results and findings were used to correlate findings and resultant values with previous researches which indeed show similar patterns for surface energies and contact angles. Refining the meshes further reduces the area for greater number of iteration steps along with a reduction in volume.

The relation between an optimized surface volume and energy along with specific contact angles have been imported to the SE-FIT extension discussed further in the paper. The graphs above show the relation to the surface energies and angles which affect the final shape of the sessile drop. As indicated, with larger angles, the energies increase to a limit. The findings were seen to correlate in terms of physical effects from previous studies and further indicated that surfactant addition to sessile drops (a similar case of hydrophobic and hydrophilic surfaces) results in a gradual drop of the surface energy coupled with a falling surface area that completely suppresses the droplet. [6]

4. MODEL VALIDATION

The validation of the models obtained from ANSYS Fluent were conducted in two ways - one that related the shapes and contours to findings in literature readings for the software [2]. The other method was by taking the parameters that were obtained from the ANSYS Fluent simulations and applying them in other settings which confirmed the shapes and structures of the zones of influence in the studies.

The parameters defined by the temperature, pressure, model type, concentration of substances and shape size were extracted from simulations that converged completely to the extent of proper phase separations, as seen in Figure 4 and Figure 7. To illustrate these effects the models for Eulerian, convective and conductive flows were used in MATLAB FEATools which confirmed the dynamics of phase separations and phase movements with time.

Figure 11 Optimization of shape specifics in SE-FIT.
Literature data suggests that under the predefined conditions set during a simulation run, the presence of Marangoni flow vectors become more apparent as the velocity vectors charge over heavier components (in this case water). Mixing studies with evaporative models were confirmed using the MATLAB models as well as the use of the SE-FIT environment (as seen in Figure 11) where the energy of the droplets was optimized as per the shape of the components to yield similar results.

These findings show that evaporative flux models with constant heat coefficients yield the most stringent parameters for showing the effects of the coffee stain effect. Further validations for the results were obtained by creating a semi-circular model influenced by the quadrant shape for ANSYS Fluent.

The shape and position of the vectors was obtained with similar conditions and separations caused by the movement of water and air components. Once again, the presence of counteracting swirling motions of the Marangoni effect revealed that such motions help in suppressing the shape of the sessile droplet [7].

**ENERGY SLAB 2D MODEL**
The software was used to study the contours of heat flux and velocity caused by varying the temperatures of the environment, the drop and the slab on which the drop is placed.

The Energy Slab 2D model was created in conjunction with the ANSYS Fluent setup with a droplet on a heating slab to mimic the environments of a sessile droplet being subjected to an evaporative heat flux. Neumann constant heat flux boundary conditions were set for the slab and the environment. The figure clearly shows the erratic velocity vectors shown later in the simulation where the temperature profile increases and reaches a constant profile after which the droplet reduces in size. The boundary in contact with the slab acts as a wall while the outer curve was set to an outlet velocity boundary condition.

Simulations show that the contour lines for the drop extended beyond that of its initial radius as the temperature of the slab was increased and heat transfer coefficients for the drop material was increased.

Velocity vectors and heat flux pathlines were observed as well, which showed the action of the drop's surface energy in flattening it and spreading it.

![Figure 12 Drop on a heating slab in Energy 2D.(Temperature-373 K and 1 atm Pressure with Eulerian Model)](image)

The Figure 12 represents the contour diagrams for velocity profiles in a magnified section of the drop surface. As time proceeds, temperature and heat flux profiles at the regions of movement become more active and act to concentrate the flow at a single point. Minor simulations studies also used the same resultant parameters from the ANSYS Fluent system which indicates that the models developed were indeed sound and congruent to realistic definitions. The formation of swirling eddies is another indication of this congruency.

All these models have been set to parameters as per the studies from literature that places data from Eulerian, constant heat flux and inviscid flows to be the most exact for replicating coffee stain effects.
The FEATool package when coupled with QuickerSim in MATLAB provides an environment to study design flow systems with boundary conditions and initial set points. The following images show the system dialog box where the environmental properties are defined along with meshing, layering and phase interactions. The software package played a decisive role in confirming the validation of the models obtained from ANSYS Fluent by producing similar phase change trends in timed simulations.

The Figure 18 below represents a cross cut schema of a droplet where the outer region (represented by darker shades of blue indicating the region in low velocity-air) and the middle with the inner regions (represented by yellow to red shades indicating the region in high velocity-water). With time, the outer regions close in on the center with the dependent variable $u$ which represents a constant heat addition that increases with time.

![Figure 18: Cross cut schema of a droplet](image)

The following 2D models in Figure 19 and 20 included all equations from the Heat Transfer Panel, Navier-Stokes Model for motion of the materials and a Conduction-Convection Model for transfer of heat from the drop [9]. The images shown represent environments that use the heat transfer models from the tool set with Navier stokes velocity equations in the x and y direction (0.001 cm/s). Appropriate densities and heat transfer coefficients were added through the convectiondiffusion.matlab functions.

Boundary conditions were set to keep the bottom as a wall with no slip condition intact and the outer curve to have a normal atmospheric outlet pressure. Temperatures were initially set at 100 degrees for the bottom with surroundings at 110 and included a gravity model with velocity acting towards the centre. Final temperatures were reached to 425 K. However, the lack of animation schemes in FEAToolBox only allowed for studying the changes by examining the system after each simulation.

5. RESULTS AND DISCUSSION

The impact of the coffee stain effect has been subsequently made in a few situations with a goal to additionally arouse into the general powers and elements that influence the spread and stream of the drops on surfaces. As evidenced by the simulation results, there have been similar results that have been created with similar environments with congruent parameters which proves to be a great method of studying the effects [10]. Pressure effects and temperature changes show and confirm that there does exist a peak condition where a clear demarcation occurs which can be best seen with the Eulerian case.

The essential goal was to make such situations inside ANSYS Fluent which have been observed to be harmonious to the impacts examined. A noteworthy takeaway remains the impact of Marangoni stream vectors on the drops which have been controlled to lessen the spread.
Different situations, for example, Surface Evolver were utilized to discover a relationship between the formed surface edges and the surface energies for characterized temperatures and weights. The figures Figure 8 and Figure 9 demonstrate the fundamental reenactment consequences of including a water vapor part under the segment segments and the collaborations that happen between the blend stage under high temperatures reliable with the profound stashes that have been believed to be framed in such environments.[11]

On contrasting the Figure 12 and Figure 13, we can surmise that static temperature for the locale remains almost equivalent however with a general drop as the blend stage (spoken to by lighter blue hues) assumes control over the exhausting water and water vapor phase (represented by light and dim yellow hues) until the point that an equivalent temperature is accomplished all through the drop that stifles any fluid segments. These discoveries associate to the elements and stage changes as concentrated by past researchers, especially in droplet simulations for ANSYS [2].

6. CONCLUSION

The dynamics and mechanisms of the coffee stain effect have been highly debated in literature as to the influence they have on the shapes and movements of particles in droplets. These mechanisms have extensive industrial applications for helping manufacturers devise methods to counter the forces producing stains and unwanted colorings on materials such as clothing.

The extra programming projects and stages were utilized to affirm the setups utilized and deliver comparative outcomes, for example, FEA and Energy2D. The Figure 6 shows and affirms that the best impacts of weight are seen at the focal plan of the drop work where the shapes diminish step by step with time, encouraged by a negative pressure (represented by the lighter and darker blue shades) at the limits of the drop [12]. These validate the impacts of weight in a multiphase bubbling case with three stages.

Additionally, a closer examination at the velocity vectors show how the more grounded speed vectors (represented by shades of blue) begin from the highest limit of the drop and travel the distance to the center with a well demarcated separation (seen by shades of red) which loan proof to the cross-sectional developments of blend segments inside the limits of the contours [13].

Contrasting Figure 4 and Figure 5 with Figure 13, we can see the comparable aftereffect of blend associations in the FEATools MATLAB condition alongside the dynamic particulate shapes made after some time. The variable u is made reference to the temperature T which is a testimony to the effects seen in literature for unsteady state effects for temperamental state conditions [14]. The resultant reenactment at last demonstrate the drop being totally recorded with water vapor however requires higher temperatures and additional time as prove when take to land at the state in the figure. Such validations were carried out by comparing the static change in phase separations and interpreting the forces driving them [14].

Progressing research is currently centered around building up a crude wellspring of information for some parameters, for example, contact edges, stage focuses, temperature and evaporative transitions, densities and mass exchange coefficients to locate the appropriate point where Marangoni stream legitimately annihilates the outward stream of the drop.

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