doi:10.2533/chimia.2013.291

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Fachhochschulen – Hautes Ecoles Spécialisées

## Modeling and Validation of Heat and Mass Transfer in Individual Coffee Beans during the Coffee Roasting Process Using Computational Fluid Dynamics (CFD)

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*Abstract:* Heat and mass transfer in individual coffee beans during roasting were simulated using computational fluid dynamics (CFD). Numerical equations for heat and mass transfer inside the coffee bean were solved using the finite volume technique in the commercial CFD code *Fluent*; the software was complemented with specific user-defined functions (UDFs). To experimentally validate the numerical model, a single coffee bean was placed in a cylindrical glass tube and roasted by a hot air flow, using the identical geometrical 3D configuration and hot air flow conditions as the ones used for numerical simulations. Temperature and humidity calculations obtained with the model were compared with experimental data. The model predicts the actual process quite accurately and represents a useful approach to monitor the coffee roasting process in real time. It provides valuable information on time-resolved process variables that are otherwise difficult to obtain experimentally, but critical to a better understanding of the coffee roasting process at the individual bean level. This includes variables such as time-resolved 3D profiles of bean temperature and moisture content, and temperature profiles of the roasting air in the vicinity of the coffee bean.

**Keywords:** Coffee roasting · CFD · Heat and mass transfer · Modeling

### 1. Introduction

Coffee is one of the main agricultural commodities traded in international markets, as well as one of the most consumed beverages globally. From the seed to the cup, coffee goes through a large number of agricultural, physical and chemical transformations. Possibly the most significant and dramatic processing step in this long chain of transformations is roasting. Indeed, roasting is a highly complex, heat and time dependent process where the typical organoleptic properties of coffee (taste, odor and color) are generated. While it is of such outstanding importance to the flavor and quality of the final brew, the dynamic processes taking place in the individual beans are still little understood. Hence roasting is currently as much art as it is science.

The roasting process can roughly be divided in two stages: the first one is the drying, where the bean temperature is below 433 K (160 °C) and the second one the actual roasting, when bean temperature is between 433 K (160 °C) and 533 K (260 °C).[1,2] During the second stage pyrolitic and polymerization reactions, among others, take place, which on the one hand fundamentally change the texture and consistence of the bean material, making it brittle (for grinding) and extractable, and on the other hand generate a large number of flavor compounds. Besides flavor, these reactions also produce non-organic volatile compounds such as water steam, carbon monoxide and carbon dioxide, the latter being the most produced gas during roasting.[3] The quantity of carbon dioxide may depend on variables related to the variety and post-harvest treatment, but most significantly is dependent on roasting conditions.[4]

In order to monitor progress of the roasting process, a large number of variables can potentially be monitored.[5–16] These include the bean temperature (more precisely: the temperature gradient from the bean surface to the center of the coffee bean), color, weight/mass loss, odor, taste, chemical composition and more.[17–20] Among all these, three are of particular importance for a better understanding and optimization of the coffee roasting process, as they form the basis of most of the chemical and physical transformations and reactions taking place inside the coffee beans. These are the bean temperature and moisture content as well as the roasting gas temperature.[21–23] A good control of the hot air temperature and roasting time can guarantee constant final product quality, provided that green coffee beans quality does not vary.[24]

In this work we have analyzed heat and mass transfer phenomena during coffee roasting at the individual bean level. For this aim, computational fluid dynamics (CFD) was used to generate flow and roasting simulations. CFD provides numerical solutions of the laws governing fluid dynamics for a given time-dependent flow process and geometry. The complex set of partial differential equations is solved in geometrical domains divided into small volumes, commonly known as a mesh or grid (control volumes). To validate the mathematical model and the outcome from the simulations, the results were compared to experimental data. The aim is to develop a useful tool for a better understanding and control of the coffee roasting process, ensuring, in a long-term objective, high and consistent quality of roasted coffee.

### 2. Material and Methods

#### 2.1 *Model Geometry*

A semi-elliptical coffee bean with axis lengths equal to the average values measured by a digital measurement device on 50 Arabica coffee beans was designed with *Design Modeler Tool* provided by ANSYS-Fluent (*www.ansys.com*) and placed with the same tool inside a cylindrical glass tube simulating the coffee roaster. The geometric values used to simulate the bean were as follows: Longitudinal diameter of the bean: 0.0098 m; equatorial diameter: 0.007 m; thickness: 0.0037 m; glass tube 0.20 m length and 0.0254 m diameter (Fig. 1).

#### 2.2 *Grid (Meshing Tool)*

An unstructured mesh containing 167507 tetrahedral elements was generated (Fig. 2). The mesh was refined up to a level where further refinement did not improve the results; (*i.e.* convergence

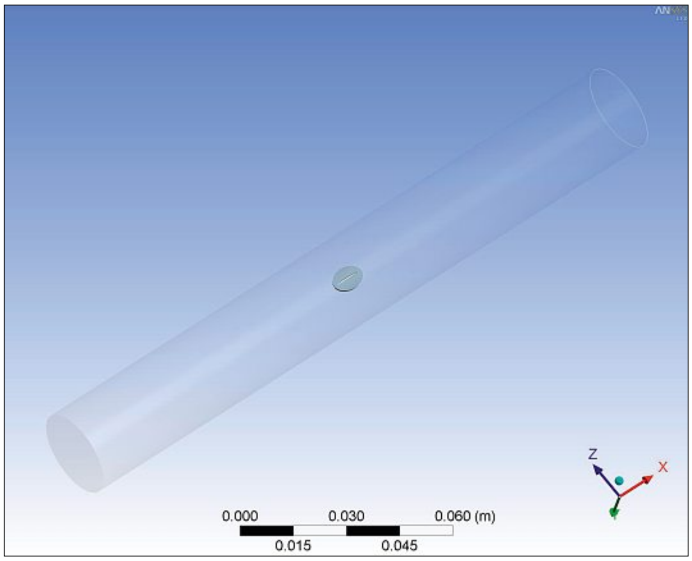


Fig. 1. Model geometry. For the mathematical simulations, a cylindrical tube was used for the roaster geometry, so as to reflect as close as possible the roasting experiments on the single bean. The coffee bean was placed at the center of the tube and roasted by a flow of hot air.

was reached), with the meshing tool provided by the software. Two significant advantages of the unstructured mesh capability in ANSYS-Fluent are:

- Reduced setup time compared to structured meshes.
- Ability to incorporate solution-adaptive refinement of the mesh.

By using solution-adaptive refinement, cells can be added where they are needed in the mesh, thus enabling the features of the flow field to be better resolved. When adaption is used properly, the resulting mesh is optimal for the flow solution because the solution is used to determine where more cells need to be added. Thus, computational resources are not wasted by the inclusion of unnecessary cells, as it occurs in the structured mesh approach. Also, the effect of mesh refinement on the solution can be studied without completely regenerating the mesh.

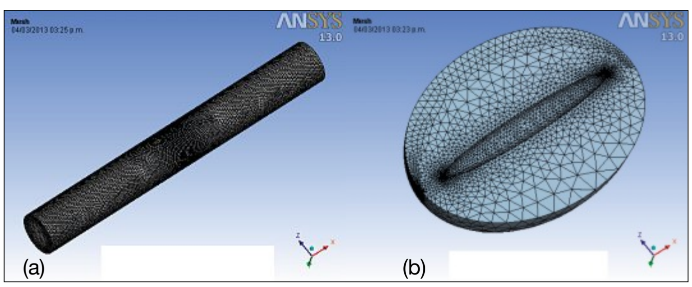


Fig. 2. Mesh for (a) the glass tube and (b) the coffee bean.

### 2.3 *Model Parameters*

Parameters listed in Table 1 were used for the simulations. The model proposed by Schwartzberg[19] was applied to describe heat and mass transfer during coffee roasting, using hot air as roasting mean. The following equations were programmed and added to ANSYS-Fluent as UDFs:

The mass loss in the coffee bean is given by Eqn. (1).

$$-\frac{dX}{dt} = \frac{4.32\times10^{9}\cdot X^{2}}{d_p^{2}}\exp\left[-\frac{9889}{T_b}\right] \quad (1)$$

Temperature change of the coffee bean with time is given by Eqn. (2).

Table 1. Model parameters: The following parameters were used for the simulations.

| | |
|---|---|
| Air temperature | 473–523 K (200-250 °C) |
| Air velocity | 2 m/s |
| Roasting time | 180–600 s |
| Heat capacity (air) | User defined function (UDF) |
| Heat capacity (coffee bean) | User defined function (UDF) |
| Moisture content (bean)[a] | Proposed by Schwartzberg (21) |
| Bean volume | Constant |

[a]Humidity content – moisture diffuses towards the product surface and evaporates only at the surface

$$\frac{dT_b}{dt} = \frac{GCp_a\left[T_{ae} - T_{as}\right] + m_{bs}\left(Q_r + \Delta H_{vap}\frac{dX}{dt}\right)}{m_{bs}\left(1+X\right)Cp_b} \quad (2)$$

$\Delta H_{vap}$ was calculated using the Regnault equation.[25]

The difference $[T_{ae} - T_{as}]$ was calculated with an air temperature proposed by Schwartzberg, with $A_{ab}$ = 1.22×10$^{-4}$m$^2$,[19] using Eqn. (3).

$$\left(T_{ae} - T_{as}\right) = \left(T_{ae} - T_b\right)\left(1 - \exp\left[-\frac{\alpha A_{ab}}{GCp_a}\right]\right) \quad (3)$$

Global heat transfer coefficient between air and coffee bean was calculated using Eqn. (4),

$$\alpha = \frac{h_e}{1 + 0.3 * Bi} \quad (4)$$

where $h_e$ was calculated using the Ranz-Marshall correlation.[26] Bean specific heat capacity was calculated by Eqns (5) and (6).[19]

$$Cp_b = \left(1.099 + 0.0070 * T_b + 5.0 * X\right)/\left(1 + X\right) \quad (5)$$

and

$$Q_r = A * \exp\left[-\frac{H_a}{R_g\left(T_b\left(°K\right)\right)}\right]\left(\frac{H_{et} - H_e}{H_{et}}\right) \quad (6)$$

Using the following parameters from Schwartzberg:[19] $(H_a/Rg)$ = 500 K, $A$ = 116200 (kJ/kg$_{\text{coffee dry 0}}$ s) and $H_{et}$ = 232 (kJ/kg).

## 3. Results and Discussion

### 3.1 *Computational Fluid Dynamics (CFD)*

In the following, first the three key results from the computational simulations are discussed. These are subsequently validated based on experimental data.

First, air velocity profiles were obtained, representing momentum transfer as a transport phenomenon during movement of roasting air going towards the coffee bean. Fig. 3 shows the development of this profile. The blue area in the middle represents the coffee bean and the red fields near the top and button surfaces of the bean are turbulence zones. The closer the air is to the bean, the higher the velocities are in these zones. The blue lines are at the tube walls, where there is no air movement.

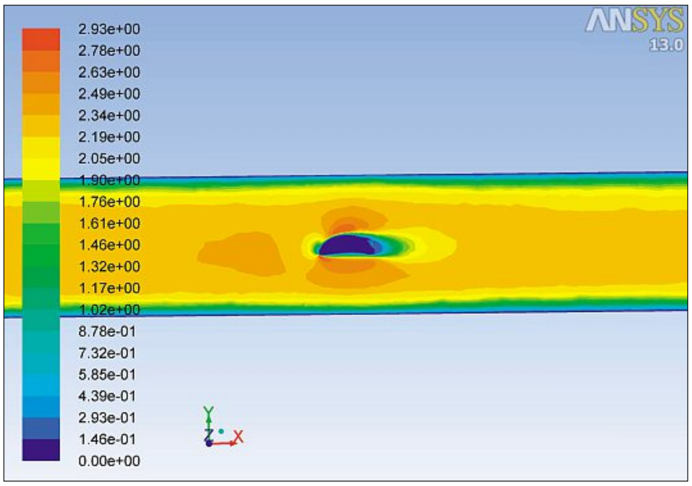


Fig. 3. Velocity profile of the roasting air at 300 s. The direction of the hot air flow is from left to right. The colour code on the left represents the velocity scale in m/s.

Second, the temperature profile for the roasting air at t = 300 s and a hot air temperature of T = 503 K (230 °C) is showed in Fig. 4. The red fields are the warmest zones at the inlet with a temperature of 503 K (230 °C). As air flows through the glass tube towards the end, the temperature decreases until it reaches the lowest value of 450 K (177 °C) at the outlet (yellow zone).

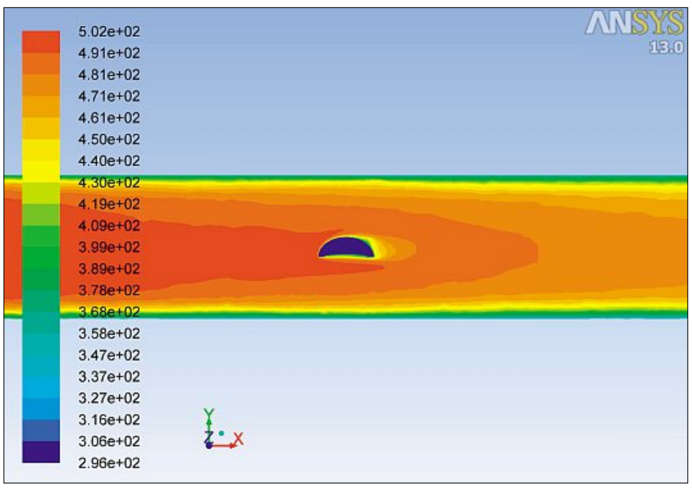


Fig. 4. Inlet air temperature profile at t = 300 seconds. The hot air roasting temperature is T = 503 K. The colour code on the left represents the temperature scale in Kelvin.

Third, bean surface temperature profile is computed. Bean temperature is a very important parameter affecting quality of roasted coffee. Fig. 5 shows the temperature profile on the bean surface after 180 seconds of roasting, for a roasting with a hot air temperature of T = 503 K (230 °C). By this time, the bean core has reached a temperature of 489 K (216 °C), while the bean surface already has a temperature of 505 K (232 °C). Hence there is a difference of 16 K between the bean core and its surface.

### 3.2 *Model Validation*

Experimental data from Rodrigo Pliego-Solórzano for bean temperature and Stefan Schenker for humidity loss were compared with CFD model results.[27–29]

A comparison of coffee bean surface temperature (experimental) with the one obtained using the CFD simulation without heat loss due to the equipment and surroundings is shown in Fig. 6 for roasting temperatures of 473 K (200 °C) and 523 K (250 °C). At the lower temperatures (473 K, 200 °C), a better match between the experimental results and the corresponding simulation were obtained, while by increasing roasting temperatures the simulation becomes slightly less accurate. A possible explanation for this behavior could be that for higher roasting temperatures (>503 K, 230 °C), coffee beans experience exothermic chemical reactions and carbonization reactions are initiated. Such major chemical transformations have not yet been considered within the model. Furthermore, the CFD simulations do not allow for an increase of bean volume during roasting.

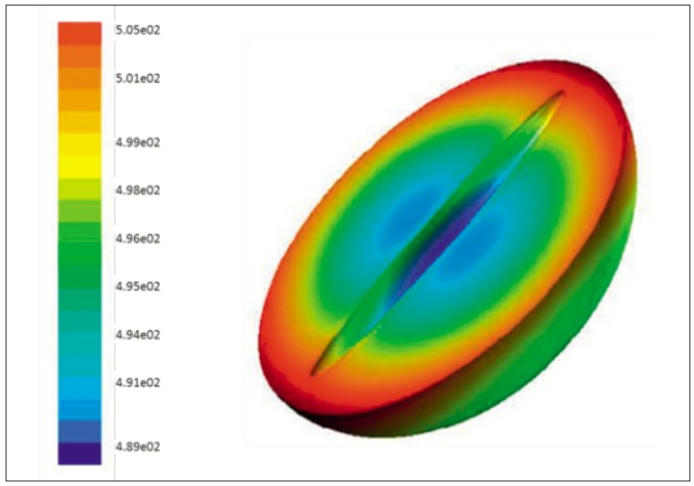


Fig. 5. Bean surface temperature profile after 180 seconds of roasting at T = 503 K hot air roasting temperature. The colour code on the left represents the temperature scale in Kelvin.

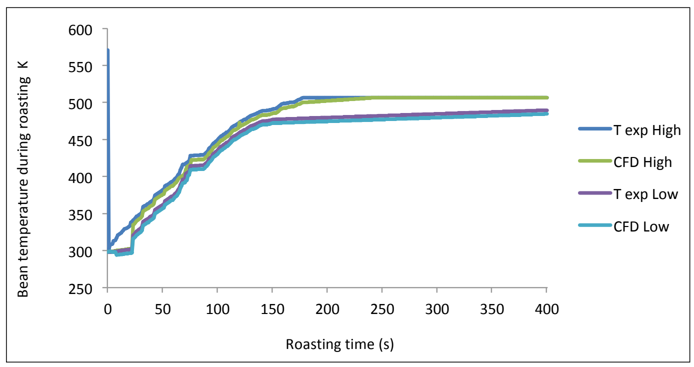


Fig. 6. Comparison between experimental coffee bean temperature and results from CFD simulations at two different roasting temperatures (200 °C, 473 K and 250 °C, 523 K).

Fig. 7 shows a comparison of the experimental outlet air temperature and the corresponding simulation with CFD. Being able to predict this temperature is important, since it can be used to estimate bean temperature and therefore to estimate its quality as well. In particular, this temperature is rather straightforward to measure, even on industrial-scale roasting facilities. The outlet air temperature for both roasting temperatures (473 K, 200 °C, low temp and 523 K, 250 °C, high temp), as time increases, shows that the simulation agrees even better with experimental data for the case of high temperature. For the low temperature a constant difference of approximately 8 K can be seen from the curves.

### 3.3 *Moisture Loss*

Experimental data from Stefan Schenker were compared with CFD simulation on humidity loss for the coffee bean.[29] Agreement was found between the two curves shown in Fig. 8, since the trend on the curves is the same. Fig. 8 (red curve) agrees well with the data measured in the dissertation of Stefan Schenker and shows a water content of about 2 g of water per 100 g of matter. At a roasting time of 300 seconds there is a difference of about 1g $H_2O$/100 g on a wet basis. The reason could be that the model does not consider the moisture content of the roasting air.

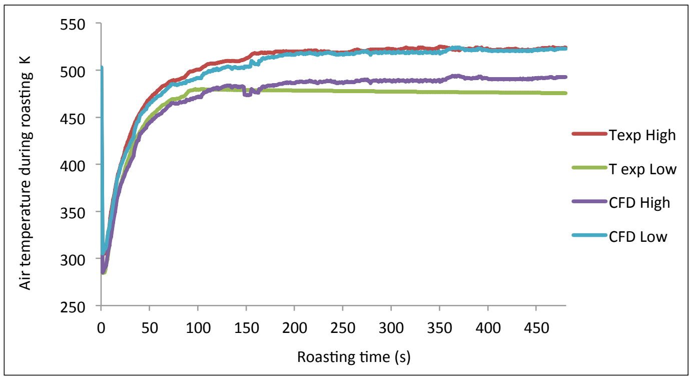


Fig. 7. Comparison of the experimentally determined air temperature (device outlet) with results from CFD simulation at two different roasting temperatures (200 °C, 473 K and 250 °C, 523 K).

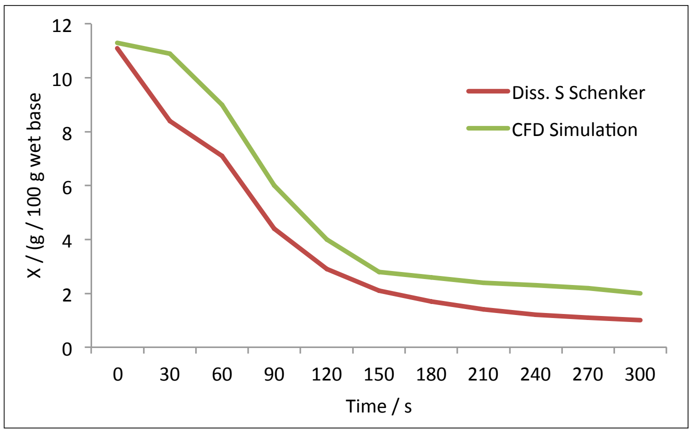


Fig. 8. Development of bean water content (x) during isothermal roasting at 260 °C hot air temperature. Comparison of experimental data from Stefan Schlenker[29] at 260 °C hot air temperature on C. Arabica, Costa Rican beans with CFD simulation in this work.

## 4. Conclusions

In this work, an evaluation of a simulation using CFD to estimate surface coffee bean temperature, hot air temperature of the roaster and moisture loss on a coffee bean was carried out. These parameters are directly related to product quality. The model for heat and mass transfer during roasting of a coffee bean was presented and validated with experimental data from different sources. Results show good agreement between simulated and experimental temperature and moisture (humidity) data. Deviations found between experimental and simulated data are due to the fact that the model does not consider all possible factors affecting moment, heat and mass transfer. Hence, a useful tool to predict coffee bean temperature and its time evolution during roasting is available, complementing and extending current methods to monitor and evaluate the impact of roasting parameters on the quality of roasted coffee.

**List of symbols**

$A$ Arrhenius equation pre-factor (kJ/kg$_{M.S}$·s)
$A_{ab}$ Contact surface between air and coffee bean (m$^2$)
$Bi$ Biot number
$Cp_a$ Air specific heat (J/kgK)
$Cp_b$ Bean specific heat (J/kgK)
$d_p$ Effective diameter of the coffee bean (m)
$G$ Air mass flow (kg/s)
$h_e$ Heat transfer coefficient at the interface between air and coffee bean (W/m$^2$K)
$H_a$ Activation energy
$H_e$ Amount of heat produced from beginning of roasting process to time $t$ (J/kg$_{M.S}$)
$\Delta H_{vap}$ Heat transfer coefficient between equipment and environment (J)
$m_{bs}$ Energy exchange surface between air and bean/pipe meters (kg)
$Q_r$ Exothermic heat production rate
$R_g$ Ideal gas constant
$T_b$ Internal coffee bean temperature
$T_{ae}$ Inlet air temperature
$T_{as}$ Outlet air temperature
$X$ Water concentration at coffee bean
$\alpha$ Global heat transfer coefficient between air and bean

***Acknowledgements***

The present work was only possible thanks to the financial support of Bühler AG. The authors would also like to thank Alexia N. Glöss and Flurin Wieland for their inputs and helpful discussions.

Received: February 3, 2013, revised: March 5, 2013

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