Lattice gas and Lattice Boltzman for spatio-temporal simulation of gases in fruit storage chambers

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KEYWORDS: gas flow, physiological processes, modelling, controlled atmosphere, simulation

ABSTRACT

The benefit of controlled and modified atmospheres for extending the storage life of fruits is world wide accepted. However, there are secondary effects such as the incidence of anaerobic respiration or the off-favour occurrence which are not sufficiently known and thus controlled. This study approaches the knowledge of those secondary effects by developing a spatio temporal model gathering fluid flow phenomenon and physic and physiological processes. The lattice Boltzmann model used as framework for mimicking the fluid flow shows to be a very flexible tool which reproduces complex macroscopic behaviours on a down up strategy better than Lattice Gas Cellular Automata (LGCA).

INTRODUCTION

Fluid Dynamics can be modelled through the Navier-Stokes equations, and there are commercial software packages available to do so (Computational Fluid Dynamics, CFD). The Navier Stokes description corresponds to a macroscopic definition of the fluid motion phenomena, however it is not the unique method to be used.

During the past 20 years new simulation procedures are emerging from Statistical Physics and Computer Science domain. One of them is the Cellular Automata (LGCA) method. This procedure corresponds to a microscopic definition of the world. The concept here is to simulate complex macroscopic (global) behaviours by means of the definition of a limited number of rules operating at a microscopic (molecular) level. For LGCA both space and time are defined as discrete variables. Space is defined in a lattice were each cell is connected to its nearest neighbours (4 or 6 depending on the lattice topology). Time is considered in two steps: movement of particles inside and between cell respectively. When appropriate, the rules defined for both steps enable to reproduce gas diffusion in a realistic way. All cells are updated simultaneously for all the lattice (Wolf-Gladrow, 2000).

Another simulation procedure for mimicking the fluid motion phenomena is the so called Lattice Boltzman method (Rothman and Zaleski, 1997). This corresponds to a meso-scale description of the world (Van Der Sman, 2001). In this case, particle distributions rather than isolated particles are considered. At each time step a collision

factor is computed (Ω) for each cell which is used to update the particle distributions at every cell of the lattice simultaneously. Simulation of laminar and turbulent motions of fluids specially when considering several gas species is still an ongoing research (Shan and Chen, 1993).

Micro and meso-scale based methods correspond to a down-up strategy while macroscopic simulation through CFD is considered an up-down procedure (Wolf-Gladrow, 2000). The main advantage of the former compared to the latter relays on facilitating the incorporation of complementary chemical and physiological phenomena to the simulation. This fact is a major issue when considering the storage of agricultural products such as fruits and vegetables.

Nowadays, the use of controlled (CA), Low Oxygen (LO) and Ultra Low Oxygen (ULO) atmospheres has been recognised as a reliable method to extend the storage life of fruits and vegetables. However, small spatial gradients in gas concentration during storage may generate internal disorders in the commodities. The accumulation of non traceable factors such as intra-batch variations in the maturity stages of the fruit and/or local lack of uniformity in the air motion, lead to the erratic occurrence of internal disorders.

The development of tools to facilitate the study of such erratic behaviours will be faced in this paper by simulating transpiration, respiration, diffusion and ventilation inside fruit storage chambers within micro and meso-scale strategies.

METHODS

Four different gases have been considered for modelling transpiration respiration and ethylene emission: oxygen, carbon dioxide, water vapour and ethylene. Transpiration affects the level of water vapour, respiration modifies both oxygen and carbon dioxide concentrations, and ethylene emission affects the concentration of this phyto-hormone in the air.

Psychometric model

The ASAE model (ASAE, 1983) is used for establishing the vapour ratio (g/kg dry air) based on relative humidity, temperature and atmospheric pressure.

Transpiration model

The water loss of the fruit towards the surrounding air is considered, due to the difference in water potential between each piece of fruit (ψ_f) and the ambient. The water potential of the air (ψ_0) is a function of the temperature (T) and the relative humidity (RH). The water potential of the fruit (ψ_f) is considered in a first approximation strictly dependent on the osmotic potential of the fruit ($\psi_{\pi f}$), and thus related to the concentration of solutes in the juice (De Smedt, 2000). For such transpiration model, the relative humidity term referred to the global relative humidity of the ambient since no spatial effect was considered. At current stage, the relative humidity for the boundary layer of the skin for each fruit is computed, which changes according to the diffusion and transport phenomena modelled with LGCA or Lattice Boltzmann.

$$\Psi_{fruit} \sim \Psi_{\pi} = \frac{RT}{V_M} Ln\left(\frac{W}{W+H}\right)$$

Eq.1

$$\Psi_0 = \frac{RT}{V_M} Ln\left(\frac{HR}{100}\right)$$

Eq.2

Respiration model

Respiration refers to hexose consumption (C_6H_{12}) by means of oxygen (O_2) which generates water vapour (H_2O) and carbon dioxide (CO_2). This process together with transpiration has already been faced in previous studies (De Smedt, 2000) miss-regarding spatial effects. Respiration decreases the osmotic potential inside the fruit and thus facilitates transpiration. Whenever the carbon dioxide in the air reaches a certain threshold (species and variety dependant) anaerobic respiration may occur leading to abnormal storage features in the fruits. The chemical reaction for respiration allows a proper calculation of mass conversion between all those chemical species.

Definition of simulated media

To proceed with the simulation of gas motion, there is a need of defining the properties of the different media: air, recipients (boxes and pallets) and fruits. Thus, in the air cells only motion phenomena may occur, recipients are considered non porous, that is impermeable cells unless perforated. Concerning the fruits, the physiological activity is concentrated towards the skin, while the inner part is considered similar to the boxes. Beside the mentioned dominia when trying to simulated forced air flows, two new dominia were also defined: suction area and fan. There is a direct mass transfer between the suction areas and the fans. Also the impulsion direction is tuneable.

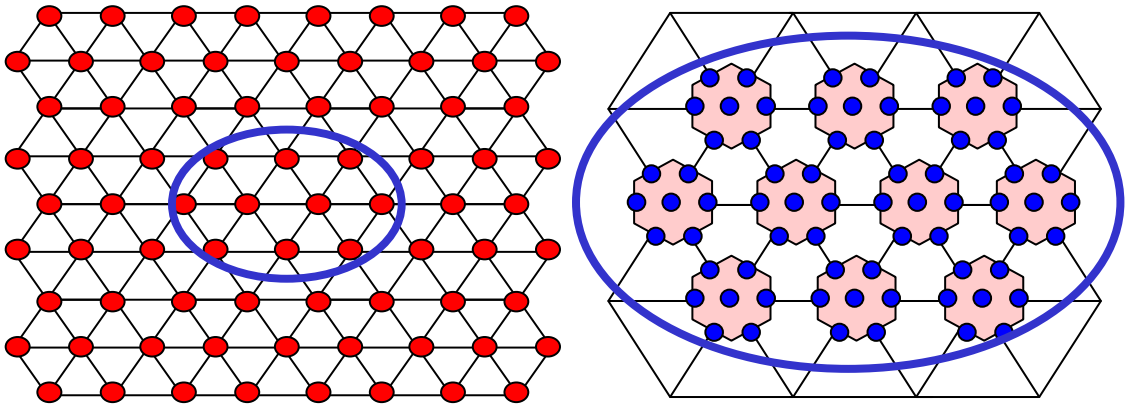

Figure 1. Hexagonal topology used for the simulation of gas motion. The figure to the right indicates the maximum number of gas particles allowed for the LGCA model.

Gas motion with LGCA

This procedure allows a proper definition of the diffusion process inside the cold storage chamber, while fails to reproduce forced air motion due to particle density restrictions inside the cells. Figure 1 shows the configuration of a hexagonal topology of the spatial lattice. Inside each cell, seven particles may concur . As stated in the previous paragraph, movement occurs in two steps: diffusion inside and between cells.

Gas motion with Lattice Boltzmann

The model proposed by Shan and Chen in 1993 demonstrates the feasibility of reproducing large range of Reynold numbers. Moreover, it enables to consider the behaviour of multiple mixable gas species. In this procedure particle distributions (n_a^{σ}) are considered instead of isolated particles as for the LGCA model. At each time step a collision factor is computed (Ω_a^{σ}) for each cell which is used to update the particle distributions at every cell of the lattice simultaneously. An overview of eq. 1 to 10 indicates that the speed (u) is computed globally for all the gas species considered weighed by mass and relaxation time of each chemical. The particle distribution in the equilibrium maximises for a direction "a" ($n_a^{\sigma(eq)}$) whenever its direction vector (e_a) is parallel to the global speed vector (u). It also increases in relation to square module of global speed (u^2). In spite of it, the particle distribution in the equilibrium at rest ($n_0^{\sigma(eq)}$) increases for increasing compressibility coefficient (d_0) and decreases in relation to square

$$n_a{}^{\sigma}(x+e_a,t+\Delta t)=n_a{}^{\sigma}(x,t)+\Omega_a{}^{\sigma}(x,t)$$

module of global speed (u^2).

$$\Omega_a{}^{\sigma}=-\frac{1}{\tau^{\sigma}}\times\left(n_a{}^{\sigma}(x,t)-n_a{}^{\sigma(eq)}(x,t)\right)\times\Delta t$$

$$n_a{}^{\sigma(eq)}(x)=n^{\sigma}(x)\times\left[\frac{1-d_0}{b}+\frac{D}{c^2b}e_a\cdot u+\frac{D(D+2)}{2c^4b}e_ae_a\cdot uu+\frac{D}{2bc^2}u^2\right]$$

Eq.3

$$n_o{}^{\sigma(eq)}(x,t)=n^{\sigma}(x)\times\left[d_0-\frac{1}{c^2}u^2\right]$$

Eq.4

Eq.5

$$e_ae_a\cdot uu=Q_{aij}\times u_i\times u_j\ \ ;\ \ i=(1,2),\ \ j=(1,2)$$

Eq.6

Eq.7

$$e_a = \begin{bmatrix} \cos(0) & \text{sen}(0) \\ \cos(\pi/3) & \text{sen}(\pi/3) \\ \cos(2\pi/3) & \text{sen}(2\pi/3) \\ \cos(3\pi/3) & \text{sen}(3\pi/3) \\ \cos(4\pi/3) & \text{sen}(4\pi/3) \\ \cos(5\pi/3) & \text{sen}(5\pi/3) \end{bmatrix}$$

$$Q_a = \begin{bmatrix} e_{a1} \cdot e_{a1} - \frac{1}{D} & e_{a1} \cdot e_{a2} \\ e_{a2} \cdot e_{a1} & e_{a2} \cdot e_{a2} - \frac{1}{D} \end{bmatrix}$$

$$u = \frac{\sum_\sigma m^\sigma \sum_\sigma \frac{n^\sigma e_a}{\tau^\sigma}}{\sum_\sigma m^\sigma \frac{n^\sigma}{\tau^\sigma}}$$

Eq.8

Eq.9

Eq.10

Figure 2 shows an example of forced air flow, where a suction area and a fan have been defined. The speed vector field is visualised after being computed with Lattice Boltzmann.

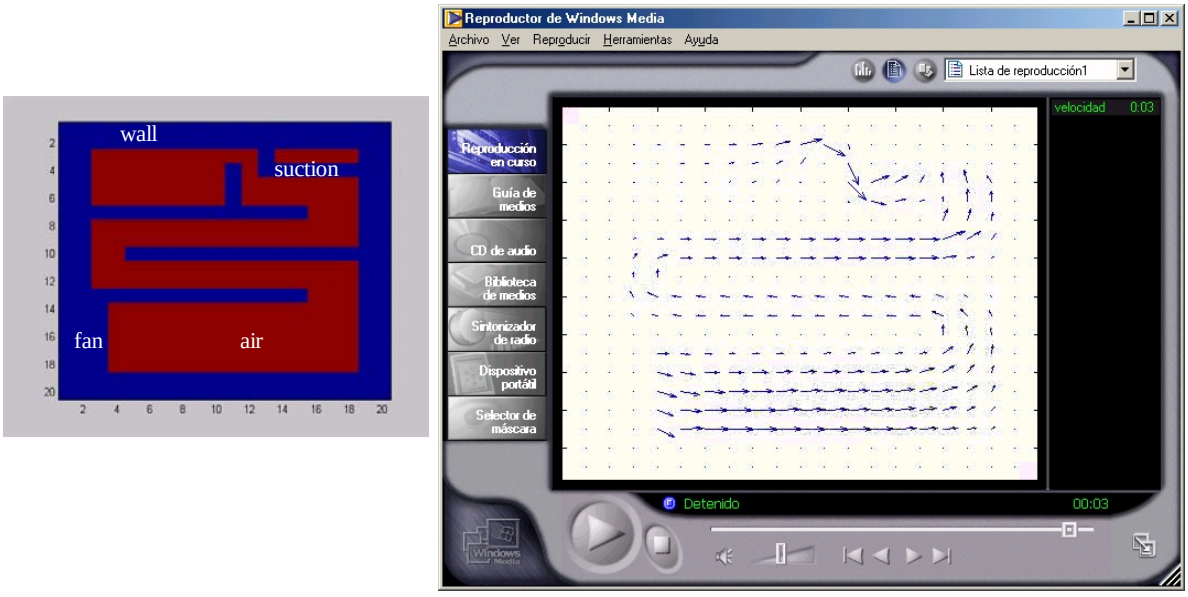

Figure 2. Example of forced air flow where a suction area and a fan have been defined. The image to the right represents the speed field computed for each cell with the Lattice Boltzmann model.

Global model

The fluid flow phenomena has been combined with relevant processes in fruit storage such as the mentioned transpiration, respiration and ethylene emission. The psychometric model defined by ASAE together with several geometric models for the

$$Voxel(\mu l / cell) = 10^9 \left(\frac{L}{512} \right)^3$$

different type of fruits are used. The definition of a scale factor (L, m) for the simulation window is basic in order to derive realistic data from draw fruits.

$$Fruit\ Mass\ (kg) = V \times \left(\frac{L}{512} \right)^3 10^3$$

$$Fruit\_External\_Surface\ (m^2) = S \times \left(\frac{L}{512} \right)^2$$

Eq.11

Eq.12

Eq.13

RESULTS OF SIMULATION

A simulation software has been implemented which combines a drawing tool with user friendly definition of the parameters of global model. Figure 3 shows the evolution of the relative humidity in the boundary layer of the fruit for two geometric models (grapes and kiwi), the fact that the relative humidity in the skin of the grapes increases at a lower rate leads to higher weight losses of the fruit. In the time evolution shown in this figure, both transpiration though the skin and diffusion to neighbour cells can be identified.

Table 1. Geometric models used for the different types of fruit in order to derive fruit mass and external surface form the drawing tool.

GEOMETRIC MODEL	TYPE OF FRUIT	PARMETERS	VOLUME (V, voxels)	EXTERNAL SURFACE (S, pixels^2)
Sphere	Apple, peach, citrus	radius, r	$V = \frac{4}{3}\pi \times r^3$	$S = 4\pi \times r^2$
Ellipsoid	Kiwi, pear	semi axes a, b	$V = \frac{4}{3}\pi \times a^2 b$	$S = 4\pi \times ab$

2/3 Toroid	Banana	radios: internal external r_1 y r_2	$V = \frac{2}{3}\pi \times r_2^{\,2} \times 2\pi r_1$	$S = \frac{2}{3} 2\pi r_2 \times 2\pi r_1$
Cone	Strawberry	radius of base, R apothem, a	$V = \frac{1}{3}\pi \times R^2 h$ $h = \sqrt{a^2 - R^2}$	$S = \pi \times R(a + R)$
Set of spheres	Grapes	number of spheres, N and radius, r	$V = N \times \frac{4}{3}\pi \times r^3$	$S = N \times 4\pi \times r^2$

Experimental data of individual fruits can be used for adjusting relevant parameters such as the mass transfer coefficient (h, mol/m^{2}Pas). The fitting procedure consists of modifying the mass transfer coefficient whenever the difference between simulated and experimental data mismatch beyond a 3% of total variance. The mass transfer coefficient is increased whenever the simulated relative humidity is lower than the experimental, and decreased on the contrary situation.

CONCLUSIONS

The flow of miscible fluids can be modelled through Lattice Boltzmann. For each cell of the lattice a overall speed is computed at each time step, which is the motor of redistribution of the particles of all the gas species considered.

The Lattice Boltzmann allows to simulate forced fluid flows. The numerical model has several parameters which are susceptible to be adjusted such as the compressibility factor (d_0) or the relaxation time for each species (τ^σ).

Different dominia may be defined easily with very different flow properties without numerical stability problems.

The fact that discrete space and time are considered enables to gather other physical (psychometric and fruit geometry models), and physiological models (transpiration, respiration, ethylene emission)

This type of simulation is a useful tool to design most relevant experiments in relation to fruit storage.

Optimisation of the computation time and increasing the lattice definition beyond 256.000 voxels remain at a research stage.

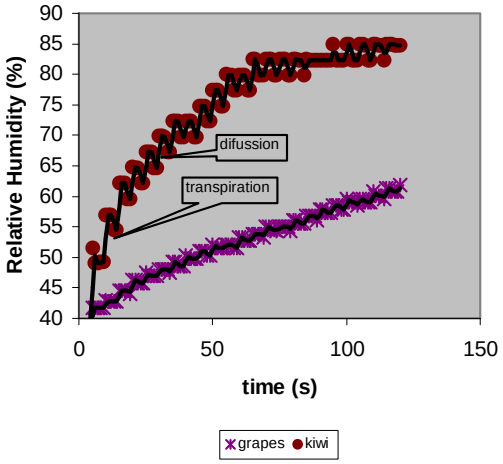

Figure 3. Time evolution of the relative humidity in the boundary layer of several fruits corresponding to different geometric models.

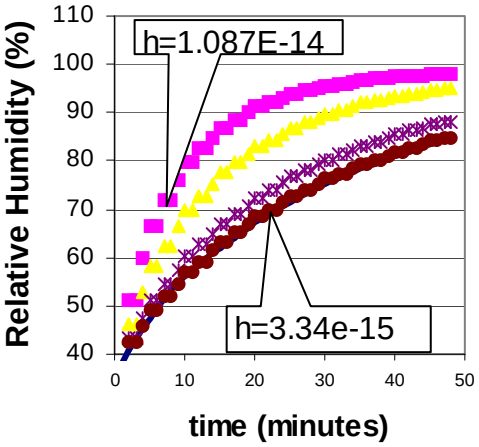

Figure 4. Adjustment of the mass transfer coefficient (h) from experimental data, 24 iterations were needed with 3.34e-15 mol/m^{2}Pas as final value.

ACKNOWLEDGEMENTS

To the Polytechnic University of Madrid for founding of the Project: Simulation of gases in fruit cold storage chambers.

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NOTATION FOR THE LATTICE BOLTZMANN MODEL

a	Spatial direction 0..6
b	Maximum number of directions (6)
σ	Chemical species (1..4)
e_a	Array of direction vectors. 6 × 2, six directions times 2 components
$\lvert e_a \rvert$	Module of direction vectors

	NOTATION FOR THE LATTICE BOLTZMANN MODEL
Δt	Time step (s)
c	Distance between cells divided by the time step considered (m/s)
n^{σ}	sum of particle densities inside a cell for each chemical species (moles)
$n_a^{\sigma(eq)}(x)$	Value of particle densities in the equilibrium (moles)
$n_a^{\sigma}(x,t)$	Particle density for each chemical species, cell and time (moles)
$\Omega_a^{\sigma}(x,t)$	Collision factor (moles/s)
τ^{σ}	Relaxation time (s)
D	Spatial dimension (2)
d_0	Compressibility coefficient (moles/moles)
u(x,t)	Overall fluid speed in a cell (m/s), two components
m	Fluid mass (molar weight, kg) for each chemical species