Porous medium modeling and parameter sensitivity analysis of 1-MCP distribution in boxes with apple fruit

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Abstract

1-methylcyclopropene (1-MCP) is a gas used commercially in cold storage rooms to delay ripening of fruit. It is currently not known how the gas distributes in the bins and is taken up by the fruit. Here a porous-medium model is developed based on volume averaging of the transport equations of momentum and 1-MCP in the air and product. The proposed model was compared with experimental data and validated direct-CFD model. The velocity field in and around the stack were well reproduced by the porous medium model. Concentration predictions were in average 4% and maximally 7% over the average measured values. The porous medium model also agrees well with the direct-CFD model. Influential model parameters were identified through parameter sensitivity study. Porosity, skin mass transfer coefficient and specific surface area

strongly affect the simulation. Accordingly model simplifications were suggested and recommended for commercial cold storage rooms.

Keywords:

Postharvest, Fruit ripening, adsorption kinetics, porous medium, CFD, cold storages

1 Introduction

1-MCP is applied in gas form as a fumigant by placing a proprietary 1-MCP release system in a room filled with produce. Through a combination of diffusion and convection the 1-MCP gas reaches the fruit and is bound on specific binding sites to delay ripening by blocking the action of ethylene (Blankenship & Dole, 2003; Sisler & Blankenship, 1996). 1-MCP is used at low concentrations (2.5 nL L^{-1} to $1 \text{ }\mu\text{L L}^{-1}$). The efficacy varies with the commodity, duration of treatment, temperature and method of application (Blankenship & Dole, 2003). To date, there is limited understanding of effective dose and distribution of 1-MCP to maximize profits in agribusiness to provide quality consumer products (Blankenship & Dole, 2003).

There are relatively few studies on the distribution of 1-MCP gas in loaded cool storage rooms. While the gas has a high diffusion coefficient (Ambaw et al. 2011), there are reasons that could cause an ineffective distribution of the gas in the cool room. First, wooden and cardboard bin and bin liner materials have a significant capacity to bound 1-MCP and can potentially reduce the active substance concentration in the air (Vallejo and Beaudry, 2006; Ambaw et al., 2011). Second, air circulation controls the convection driven distribution of the gas and could provide preferential routes while particular zones are not reached. Third, air flow may add to the rate at which the gas is transferred to the fruit and thus the rate at which the fruit is saturated by 1-MCP (Ambaw et al. 2012a). Thus, the gas transport process with the dimensions and configuration of

the cool storage room can play an important role in the efficacy of the treatment. To study the effect of these interacting factors experimentally is difficult and time consuming. Numerical models, therefore, are a valuable tool to understand and design the process. In postharvest and various other processes, computational fluid dynamics (CFD) is commonly applied as an alternative to experimental studies of convection driven problems (Ambaw et al. 2012a,b; Delele et al. 2010; Alvarez and Flick, 2007; Verboven et al. 2006; Zou et al., 2006a,b).

Inside the fruit, 1-MCP diffuses from the surface to the centre and is absorbed by target and non-target binding sites. A model that describes this diffusion-reaction process in fruit tissue and non-target solid materials was developed by Ambaw et al. (2011). This model was employed in a direct CFD model of 1-MCP applications in which the detailed geometry of apple fruit was considered (Ambaw et al., 2012a). Simulations with this direct CFD model aided the detailed analysis of the effect of design and operational factors when the number of fruit was small enough to be handled numerically by desk-top computers. Direct CFD modeling, resolving every fruit, is impractical for fully loaded cool storage rooms filled with hundreds of tons of fruit (Verboven et al., 2006). Here, dimensions range from one-tenths of a millimeter to several meters. The wide range of scales requires a large number of computational points in the numerical procedure to solve the direct CFD model, increasing the computational demand beyond the resources available today. A porous medium model using volume-averaged transport equations is hence required (Hoang et al., 2003, 2004; Nahor et al., 2005).

In the volume averaging technique, the products and the air spaces in between compose a porous domain. Every volume within the domain is assumed to contain the product (the solid phase) and the air (the fluid phase). The two phases are continuum, separated by irregular interfaces that are not resolved geometrically but parameterized through the volume averaging procedure

(Hassanizadeh and Gray, 1979). Depending on the level of simplification, one can arrive at one-phase or two-phase models (Verboven et al., 2006). The one-phase model assumes local thermodynamic equilibrium and arrives at a single transport equation, but the simplifications applied in using this approach are so severe that it usually leads to considerable errors, especially for transient problems (Lerew, 1978). The two-phase model involves volume-averaging of the transport equations over each phase to arrive at system of equations to be solved separately. The equations are coupled through interfacial conditions which are expressed as function of interfacial concentrations and interfacial fluxes. This approach is more realistic for transient problems where the local equilibrium hypothesis is not well verified (Verboven et al. 2006). The two-phase volume-averaging has been implemented for postharvest applications to solve heat and mass transfer problems, including room design and package design for optimal cooling of horticultural products (Hoang et al., 2003, 2004, Nahor et al., 2005). However, existing porous medium models of airflow and mass transfer in stacked fruits have not incorporated diffusion-adsorption phenomena.

In the present paper, the two-phase volume averaging technique is implemented to develop a porous medium model of the spatial and temporal 1-MCP distribution in cool storage rooms that take into account the gas diffusion-adsorption phenomena. A previously developed and validated direct CFD model (Ambaw et al. 2012a) allowed carrying out a detailed evaluation of the approach. A parameter sensitivity analysis is performed to study the relative importance of the model parameters.

2 Materials and methods

2.1 Fruit supply

‘Jonagold’ apples (*Malus domestica* Borkh, cv. Jonagold) were purchased directly after harvest from a local grower in Belgium in September, 2011. All the fruits used for the test were free of visual defects. Fruits were stored at 1°C in normal atmospheric air before and during the experiment that took place within a few days. The mean $\pm$ standard deviation ($n = 10$) of the mass and volume of fruits were $235\text{g} \pm 32\text{ g}$ and $281\text{ mL} \pm 36\text{ mL}$, respectively.

2.2 Experiment in the 500 L container

The experiment was designed to obtain spatio-temporal 1-MCP concentration data and spatial velocity data. For this, 80 kg fruit (in four plastic boxes, each holding 20kg) and a 1-MCP releasing system were placed together in a closed 500L container (see Fig.1). At regular intervals during a 24 hours period, gas samples were taken from eight locations and 1-MCP concentration measurement was made for each sample using gas chromatography. The times of 1-MCP concentration measurements were 2, 4, 6, 8, 10 and 24 h after closing the container. Velocity measurements were done by means of air velocity transducers from a total of twenty-five different locations inside the container. The experiment was performed in three replicates. Details of the experimental setup were discussed in our previous work (Ambaw et al., 2012a) and hence not repeated here.

2.3 Mathematical model

A two-phase porous medium model of the convection-diffusion-reaction of 1-MCP in stacks of fruit was developed using the volume averaging technique as described by several researchers (Hassanizadeh and Gray, 1979; Liu and Masliyah, 2005, Quintard and Whitaker, 2005; Whitaker,

1999) and are hence not repeated here. The general and particular assumptions taken to apply the volume averaging technique and the resulting model equations are stated below.

2.3.1 Assumptions

- Fruit loaded boxes were assumed as a porous domain consisting of a fluid phase (1-MCP-air mixture) and a solid phase (apple fruit).
- Passive scalar transport equations were used to describe the transport of 1-MCP in air. This is reasonable for the fact that 1-MCP used during treatment is extremely dilute; its effect on the airflow was, therefore, negligible.
- 1-MCP adsorption was assumed irreversible and the bound 1-MCP is assumed to be a non-convective, non-diffusive scalar variable. Unbound 1-MCP exists in the air outside the solid as well as in the intercellular pore spaces of the fruit. The transport of unbound 1-MCP in air was described by a convective-diffusive scalar transport equation and by a diffusive scalar transport equation in the solid pores. Convection-diffusion-adsorption parameters obtained from previously developed and validated models (Ambaw et al. 2011) were used.
- Isothermal conditions were assumed. Fruit was stored at 1 °C in normal atmospheric air before and during the experiment. At this low temperature, the respiration heat generation of fruit is considerably low and was neglected.
- The product is assumed homogeneous with constant properties throughout.

- The product is assumed spherical and the specific area of the packed apple fruit was estimated based on porosity and average diameter of the spheres representing the apple fruit.
- The pressure loss inside the porous medium was described by directional loss models with linear and quadratic coefficients determined from simulated pressure drop data from direct CFD model of single fruit loaded box (Delele et al., 2009).

2.3.2 Macroscopic equation of airflow

The porosity, mass conservation and momentum conservations for the porous domain are given by Eqn. 1, 2 and 3, respectively (ANSYS CFX-Solver Theory Guide), assuming constant porosity in space:

$$dV_a = \varepsilon dV \quad (1)$$

$$\nabla \cdot (\varepsilon \mathbf{U}) = 0 \quad (2)$$

$$\frac{\partial(\varepsilon \rho_a \mathbf{U})}{\partial t} + \nabla \cdot (\varepsilon \rho_a (\mathbf{U} \otimes \mathbf{U})) - \nabla \cdot \left(\varepsilon (\mu + \mu_t) \left(\nabla \mathbf{U} + (\nabla \mathbf{U})^T \right) - \frac{2}{3} \delta \nabla \cdot \mathbf{U} \right) = \varepsilon S_M - \varepsilon \nabla p \quad (3)$$

S_M in Eqn. (3) calculates the pressure loss of the flow in the porous medium. In this study the pressure loss was modeled using directional loss model as:

$$S_{M,i} = C_{R1i} u_i + C_{R2i} |\mathbf{U}| u_i \quad (4)$$

2.3.3 Macroscopic equation of 1-MCP conservation

The fluid and solid phase volume-averaged unbound 1-MCP transport equation are given by:

$$\frac{\partial(\varepsilon C_a)}{\partial t} + \nabla \cdot (\varepsilon C_a \mathbf{U} - \tau \varepsilon (D_a + D_t) \nabla C_a) + a_s h_m (C_a - C_s) = 0 \quad (5)$$

$$\frac{\partial((1-\varepsilon)C_s)}{\partial t} = -D_s \nabla^2 ((1-\varepsilon)C_s) + a_s h_m (C_a - C_s) - (1-\varepsilon)r_s \quad (6)$$

The volume-averaged bound 1-MCP equation is:

$$\frac{\partial C_B}{\partial t} = (1-\varepsilon)r_s \quad (7)$$

r_s is the rate of adsorption and was modelled by Ambaw et al. (2011)

$$r_s = k_a (C_{\max} - C_B)C_s \quad (8)$$

Values of the model parameters are summarized in Table 1 and were obtained from previous experiments (Ambaw et al., 2011).

The tortuosity τ , in Eqn. 5, is defined as the ratio of linear distance between two points (say, point 1 and point 2) both in the fluid phase to the actual length of diffusion path it takes to reach point 2 from point 1. For randomly packed beds of spheres, the tortuosity can be estimated as a function of porosity by (Liu and Masliyah, 2005):

$$\tau = \left[\frac{(0.2 + 0.8\varepsilon)\varepsilon^{20}}{\varepsilon^{13} + 1.4 \times 10^{-8}(1-\varepsilon)} \right]^{1/16} \quad (9)$$

The mass transfer coefficient between the fluid and solid phase (h_m) consists of the resistance of the apple skin mass transfer coefficient (h_s) and the air film mass transfer coefficient (h_a) and was estimated using:

$$\frac{1}{h_m} = \frac{1}{h_s} + \frac{1}{h_a} \quad (10)$$

The skin mass transfer coefficient is estimated from the effective diffusion coefficient of 1-MCP in fruit tissue and the characteristic length, which in this case is the radius of the spherical fruit

(Van der Sman, 2003). Taking the average radius to be 0.04 m, the skin mass transfer coefficient becomes $6.0 \times 10^{-7} \text{ m s}^{-1}$. The air film mass transfer coefficient is estimated from correlation equations. For Reynolds number ranging from 10 to 10000 for gases in a packed bed of sphere recommended correlation equation with an average deviation of about $\pm 20\%$ and a maximum of $\pm 50\%$ (Dwivedi & Upadhyay, 1977) is

$$J_D = \frac{0.4548}{\varepsilon} \text{Re}^{-0.4069} = \frac{h_a}{u} \left(\frac{\mu}{\rho D_a} \right)^{2/3} \quad (11)$$

For the expected velocity range inside the stack, namely 0.001 to 0.1 m s^{-1} , the air film mass transfer coefficient ranges from 2.16×10^{-4} to $3.32 \times 10^{-3} \text{ m s}^{-1}$. Clearly, this is much larger than the skin mass transfer coefficient. It can thus be expected that the uptake process by the fruit is diffusion driven rather than convection driven.

The turbulent diffusion coefficient, through the empirical turbulent Schmidt number, is a function of the turbulent viscosity ($D_t = \mu_t / \text{Sc}_t$). In all CFD models of this study the SST k- ω turbulence model was used for its superior performance over other steady Reynolds-averaged Navier-Stokes turbulence models (Delele et al, 2008, Defraeye et al., 2012).

2.3.4 Geometry and computational domains

Fig. 1a shows the geometry of the direct CFD model. The position, size and shape of the vent-holes of the boxes are explicitly accounted. DE modeling was used to generate the geometry of random stacking of 90 spheres (representing fruit) with diameter ranging from 80 to 85 mm in a box (Tijskens et al., 2003). Fig. 1b shows the schematics of the porous medium model that is equivalent to the direct CFD model. In this model, the details of the boxes and fruit were dropped and replaced by the porous domain.

2.3.5 Boundary and initial conditions

Fluid-solid interfaces were explicitly defined between the fluid and the solid domains for the direct CFD model and set to a conservative interface flux for the scalar and no slip walls for momentum transfer. In the porous medium model, fluid-porous interfaces were explicitly defined between the fluid and porous domains and set to a conservative interface flux boundary for the momentum and scalar conservation equations. In both models, internal walls of the container, external surfaces of the circulation fan and external surface of the 1-MCP generator were set to no slip walls. 1-MCP gas entering the domain was described by adding a boundary source at the surface representing the outlet of the gas generator. The source is defined by a stepwise decreasing 1-MCP flux term in such a way that 80%, 18% and 2% of the full 1-MCP dose enters the domain within the first, second and third hours respectively, and zero during the remaining period. The 1-MCP release profile from the generator was approximated from a separate experiment by placing the generator in an empty container. The initial concentration of 1-MCP in every domain in the model was equal to zero.

2.3.6 Simulation setup

Simulations were performed using ANSYS-CFX-13 (ANSYS CFX, 2010), which uses the finite volume method. The discretization and grid sensitivity studies of the direct CFD model were discussed in our previous work (Ambaw et al. 2012). For the porous medium model, the grid convergence index, which is based on Richardson extrapolation, was used (Journal of Fluids Engineering, 2008). The optimum grid consisted of 23,000 cells for each box and a total of 250,672 cells for the whole domain.

For each problem, first, a steady state calculation was performed to obtain a converged solution of the airflow. The steady state solutions were then used as initial values in the subsequent transient scalar transport calculation.

2.3.7 Parameter sensitivity analysis

The model parameters of the porous medium model are listed in Table 1. The purpose of the sensitivity analysis was to quantify the relative importance of these parameters. The outputs of interest in the present study are uniformity of the distribution of unbound 1-MCP and degree of adsorption of the gas in the porous medium at intermediate time ($t = 4\text{h}$). At this intermediate time there is some adsorption, which is anything but the saturation level, and it is within equitable computing time. Uniformity of the gas distribution is measured as the standard deviation of the local to the volume averaged unbound 1-MCP concentrations. Degree of adsorption is measured as the ratio of volume averaged bound 1-MCP concentration during 4 hours to the maximum adsorption capacity of apple fruits which is equal to $4.87 \times 10^{-6} \text{ kg m}^{-3}$.

The sensitivity study was performed in two separate groups (Group 1 and Group 2, see Table 1). Group 1 consist fluid flow parameters and Group 2 scalar transport parameters. The nominal values and value ranges of the parameters included in the sensitivity analysis are summarized in Table 1. In cases where the value range was not available or small, a range of $\pm 10\%$ of the nominal value was used.

The parameter sensitivity study was performed by using the design-of-experiment (DOE) capability of the Design Exploration tool of ANSYS Workbench. The overall numbers of tests (simulation runs) for the sensitivity analysis for each scenario were determined based on a

Central Composite Design (CCD). A total of 45 and 85 simulation runs were instigated by the CCD for Group 1 and Group 2, respectively.

3 Results and discussions

3.1 Comparison of the porous medium and direct CFD model of the storage container

3.1.1 Airflow pattern

Table 2 summarizes the linear and quadratic coefficients of the momentum loss model. The pressure drop across the single box along the three directions, simulated using the direct CFD models, are shown in Fig. 2 a, b and c for flow along +x, +y and -z directions respectively. The resistances to flow (the pressure drop per unit length) across side faces (along the x- and z-axis) are equal, whereas, the resistance to vertical flow (along the y-axis) is different and considerably higher. This is due to the small area fraction of vent holes at the bottom face of the box. The direct CFD models helped to calculate and capture the anisotropic pressure losses effectively.

Fig. 3 shows velocity contour plots (color) and velocity direction (arrows) taken on a vertical cutting plane passing through the centre of the stack. While the porous medium model predicts averaged values, the direct CFD model provides more detailed information of airflow through vent holes and in the air spaces between the fruits. The porous medium model reproduces the highs and lows of the velocity field satisfactorily.

Fig. 4 shows the horizontal profiles of velocities obtained from direct CFD model (full curves) and porous medium model (dashed curves) along with velocity measurement data (blue dots). Higher velocities outside the stack and low velocities (mostly < 0.01 m/s) inside the stack are well reproduced by the porous medium model. The special feature of the air flow in the region

above fruits in the bottom box is, however, not properly captured by the porous medium model (Fig. 4d). In this region, there is a characteristic channeled flow formed by the vent holes of the box, and the restriction due to the bottom of the top box and the fruits from below. This is due to the assumption of uniform porosity in the porous medium model.

3.1.2 1-MCP distribution

Fig. 5a depicts simulated and measured values of 1-MCP concentration as free in air in the container. Both the porous and direct CFD models predicted essentially uniform gas concentration in the air. In confirmation, the measured values were also spatially uniform. The observed spatial variability in the measurement was random with no characteristic trend and within the measurement errors. There is, though, a slight off-set error with respect to the average measured profile. The direct CFD model is, in average, 3% and maximally 5% over the average measured values. The porous medium model is, in average, 4% and maximally 7% over the average measured values. Difficulty in accurately capturing the geometry of stacked apple fruit in a box, as well as several other model assumptions contributes to the error.

Fig. 5b depicts simulated unbound 1-MCP. Experimental determination of the magnitude of unbound 1-MCP in fruit is almost impossible. The direct CFD model provides a framework to examine the accuracy of the porous medium model in predicting the unbound in fruit concentrations in time. Once more, the agreement between the two models is adequate with a maximum difference of 10% during the early stage of the process. After about 10 h the two models predicts similarly.

Concentration contours of 1-MCP that is free in air, unbound and bound in the fruit are shown in Fig. 6. The plot depicts the level of detail information that the direct CFD model can provide as

compared to the porous medium model. Both models predict a uniform 1-MCP distribution in the air (Fig. 6 top row). The porous medium model predicts average distributions of unbound (Fig. 6 middle row) and bound (Fig.6 bottom row) 1-MCP concentrations across the porous domain missing the distinct concentration gradients inside fruits. The direct CFD model calculates the gradients of the 1-MCP concentration inside individual fruits.

The computation of the unbound and bound 1-MCP concentrations by the porous medium model was to a great extent affected by the value of the mass transfer coefficient. Porous medium simulations based on air film mass transfer coefficient only leads to erroneous prediction of the bound 1-MCP concentration. Aspect of this observation is discussed below.

3.1.3 Effect of the mass transfer coefficient

Comparisons of simulated volume-averaged bound 1-MCP concentrations of the porous medium model based on air film mass transfer coefficient only (FMTC) (dash-dot curve) and air film and skin mass transfer coefficients combined (F+SMTC) (dash-dot-dot curve) are shown in Fig. 7 together with the result obtained from the direct CFD model (full curve). This plot reveals that FMTC overestimated the rate of adsorption (measured as the slope of the concentration vs. time curve) significantly. The time to reach 90% saturation is estimated as 6, 10 and 11 hours by the FMTC, F+SMTC and direct CFD models respectively. The rationale in using the air film mass transfer coefficient only was the assumption that the solid phase resistance would be captured by the solid phase volume averaged transport equation. But, in the volume averaged equation, the solid phase transport term becomes inconsequential to truly act as rate limiting. The high Biot number (> 2) of the porous medium indicates the importance of solid phase resistance. The incorporated skin mass transfer coefficient in essence corresponds to the solid phase resistance and enables the porous medium model to better capture the adsorption profile.

3.2 Parameter sensitivity analysis

3.2.1 Sensitivity with respect to fluid flow parameters

Fig. 8a and b show the result of the sensitivity study of Group 1 parameters. The strong effect of porosity on degree of saturation and uniformity of gas distribution is evident. Porosity, in addition to describing the fluid flow, also defines the amount of adsorbent (solid volume) present in the medium. The inverse relationship with respect to degree of adsorption is in accordance to the way porosity related to the amount of adsorbent in the porous domain. Higher porosity means lower adsorbent volume (resulting in high 1-MCP-to-adsorbent ratio).

The turbulent Schmidt number, the viscous and inertial coefficients of the momentum loss models has minor effects on the degree of adsorption and uniformity of gas distribution. Particularly, the sensitivity with respect to coefficients of the momentum loss model along the y-axis is negligible. This suggests the possibility of simplifying the porous medium model by assuming an isotropic momentum loss model.

3.2.2 Sensitivities with respect to the scalar transport parameters

The relative importance of the scalar transport parameters on the degree of saturation (Fig. 8c), is sequenced as: $a_s > h_s > k_s > \tau > D_a > h_a > D_s$. With respect to the uniformity of gas distribution (Fig. 7d), the parameters are sequenced as: $a_s > h_s > k_s > \tau > D_s > D_a > h_a$. The adsorption coefficient is inversely related to the uniformity of gas distribution. The specific area and the skin mass transfer coefficient have the stronger effects. These two parameters together establish the interfacial transfer; also, in essence h_s define the solid phase diffusion process. This result confirms the rate determining role of the solid phase transport process. The diffusion of 1-MCP between fruits (taken into account by D_s) does not play a significant role in the uptake and distribution process. The rather minor influence of the tortuosity and air film mass transfer

coefficient and the air diffusion coefficient are logical. These parameters characterize the fluid phase transport process which is sufficiently fast in the process. Overall, the parameter sensitivity analysis clearly shows the relative importance of the various processes in the gas transport.

4 Conclusions

A porous medium model for simulating the distribution of 1-MCP in boxes of fruit was developed using the volume averaging technique. The reliability of the approach was assessed through a thorough comparison of the porous medium model with an equivalent direct CFD model and experimental measurements. Though the porous medium model cannot capture local concentration gradients, it can be used to assess the condition of global gas distribution.

Through comprehensive parameter sensitivity analysis this work clearly showed where the influential transport processes. Fluid flow parameters were observed to have negligible influence on the simulation of the gas transport. Porosity, specific surface area, skin mass transfer coefficient, and adsorption rate constant have strong influence on the porous medium simulation. Based on this observation, one can consider model simplifications, for instance, by considering isotropic instead of directional momentum loss models and also by excluding the diffusion transport term from the volume averaged transport equation.

The results presented here are only valid for systems with similar dimensions to the 500 L container used in this study. When the dimensions are in a different order of magnitude, like in commercial storage rooms for 200 to 500 tons of fruit, the relative time constants of the different mechanisms may change and other mechanisms may become important. The study has; however, shown the validity of the porous medium model, which can now be used to study such

commercial systems. The approach developed is generic; it can be used to develop models of transport of other gases in closed rooms with corresponding adjustment of model parameters.

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418 **Nomenclature**

419 **Roman symbols**

a_s	Specific surface area of bulk apple fruits, $6(1-\varepsilon)/d$	m^2/m^3
C_a	Concentration of 1-MCP in air	kg/m^3
C_B	Concentration of bound 1-MCP in fruit	kg/m^3
$C_{\max}$	1-MCP adsorption capacity of apple fruit	kg/m^3
C_{R1i}	Linear Resistance Coefficient	$\text{kg m}^{-3} \text{ s}^{-1}$
C_{R2i}	Quadratic Resistance Coefficient	kg m^{-4}
C_s	Concentration of bound 1-MCP in wood	kg/m^3
d	Average diameter of apple fruits	m
D_a	Diffusion coefficient of 1-MCP in air	m^2/s
D_s	Effective diffusion coefficient of 1-MCP inside fruits	m^2/s
D_t	Turbulent Diffusion coefficient	m^2/s
dV	Volume of the representative elemental volume	

dV_a	Volume occupied by air phase in the elemental volume	
h_a	Air film mass transfer coefficient	m/s
h_m	Overall mass transfer coefficient in the stack	m/s
h_s	Skin mass transfer coefficient	m/s
J_D	Dimensionless factor	
k	Turbulence kinetic energy	m^2/s^2
p	Pressure	Pa
Re	Reynold number	
r_s	Rate of 1-MCP adsorption in apple fruit	$\text{kg m}^{-3} \text{s}^{-1}$
S_u	Momentum source term	$\text{kg m}^{-2} \text{s}^{-2}$
t	Time	s
$\mathbf{U}$	Vector of velocity, $\mathbf{V}_{x,y,z}$	m/s
u	Velocity magnitude	m/s

420 **Greek symbols**

ε	Porosity of stacked apple fruits given	
μ	Dynamic viscosity	$\text{kg m}^{-1} \text{s}^{-1}$
μ_t	Turbulent eddy viscosity	$\text{kg m}^{-1} \text{s}^{-1}$
μ_{eff}	Effective viscosity ($= \mu + \mu_t$)	$\text{kg m}^{-1} \text{s}^{-1}$
ρ_a	Density of dry air	Kg m^{-3}
δ	Identity matrix or Kronecker Delta function	
τ	Tortuosity	

421 **Sub and super-scripts**

a	Air	
max	Maximum	
s	Solid	
t	Turbulent	
$\mathbf{T}$	The transform operator	

Tables

Table 1 Nominal values and value ranges of the model parameters used for the sensitivity study

Group	Parameters	Nominal value	Range	Reference
Group 1	CR1x and CR1z	1.5	$\pm 10\%$	Range is assumed
	CR2x and CR2z	118	$\pm 10\%$	Range is assumed
	CR1y	267	$\pm 10\%$	Range is assumed
	CR2y	4748	$\pm 10\%$	Range is assumed
	Porosity, ε	0.5	0.4 – 0.6	Calculated
	Turbulent Schmidt number, Sc_t	0.9	0.2 – 1.3	Tominaga & Stathopoulos (2007)
	Adsorption rate constant, k_a	3.62	$\pm 10\%$	Ambaw et al. 2011
	Air film mass transfer coefficient, h_a	2.3×10^{-4}	$\pm 25\%$	Dwivedi & Upadhyay, 1977
	Diffusion coefficient in air, D_a	8.67×10^{-6}	$\pm 10\%$	Ambaw et al. 2011
	Diffusion coefficient in fruits, D_s	2.41×10^{-8}	$\pm 10\%$	Ambaw et al. 2011
Group 2	Skin mass transfer coefficient, h_s	5.5×10^{-7}	$\pm 10\%$	Pham et al. 2009
	Specific surface area, a_s	35	$\pm 10\%$	Calculated
	Tortuosity, τ	0.6	0.5 – 0.8	Liu and Masliyah, 1996

Table 2 Linear and quadratic coefficients of the airflow resistance model of the porous medium, obtained from direct CFD simulation

Direction	C_{R1}	C_{R2}
x	1.5	118
y	262	4748
z	1.5	118

Fig. 1. Schematics of the model geometry for studying 1-MCP treatment in a 500 L container: direct CFD model (a) and porous medium model (b). The model geometry considers only half of the full experimental setup by assuming symmetry.

Fig. 2. Simulated pressured drops across single box using the direct CFD model. Flow from bottom to top of the box (along y axis) (a), flow perpendicular to the smaller side face of the box (along x-axis) (b) and flow perpendicular to the larger side face of the box (along $-z$) (c). The contour is shown on a plane bisecting the stack. Superficial velocity for these particular contours was 4 m s^{-1} .

■ 0 m/s
 ■ >0.5 m/s

Fig. 3. Velocity contour and airflow direction on vertical plane (parallel to the symmetry plane) through the center of the boxes in the storage container: direct CFD model (left) and porous medium model (right).

Fig. 4. Measured (blue dots) and calculated by the direct CFD model (full curve) and porous medium model (broken curve) velocity magnitudes across the region above the stack (a), upper region inside the top box (b), middle region inside the top box (c), upper region inside the bottom box (d) and middle region inside the bottom box (e).

Fig. 5. Simulation of profiles of concentration of 1-MCP in the air (a), unbound 1-MCP in the fruit (b) using direct CFD model (full curve) and porous medium model (dashed curves). The curves are for values averaged over the boxes. Symbols in (a) are measurement values of samples. The 1-MCP dose was 1 $\mu\text{L/L}$, and the temperature was 1 $^{\circ}\text{C}$.

Fig. 6. Contour of free in air (top row), unbound in fruits (middle row) and bound in fruits (bottom row) on a vertical section through center of the boxes from the porous medium and direct CFD models at three different times.

470

471 Fig. 7. Comparison of the time dependent bound 1-MCP concentration (averaged over the boxes)
 472 calculated by the porous medium model with air film mass transfer coefficient only (dash-dot
 473 curve), air film and skin mass transfer coefficient combined (dash curve) and by the direct CFD
 474 model (full curve).
 475

Fig. 8. Bar graphs showing sensitivities of the porous medium model simulations to Group 1 parameters (top row) and Group 2 parameters (bottom row) in predicting degree of saturation (left column) and uniformity of gas distribution (right column).