Research Report

Predicting vapour and particle distribution of CIPC in potato stores

Y. Xu; P. C. H. Miller; A. G. Lane
Silsoe Research Institute

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British Potato Council
4300 Nash Court
John Smith Drive
Oxford Business Park South
OXFORD OX4 2RT

SUMMARY

(1) Preliminary experiments in which CIPC vapour was introduced into a chamber from which air samples were drawn to determine the size distributions and airborne concentrations of particles suggested that it would be possible to treat potato stores with vapour as a means of distributing CIPC more evenly within a store.

(2) A potential method of generating CIPC vapour by heating solid material to a controlled temperature in a glass container was shown to be feasible at an experimental scale.

(3) Models have been developed to predict the application of vapour CIPC for sprout control in commercial potato stores. These include models for CIPC evaporation into air, transportation by air movements and absorption by potatoes.

(4) There was no clear evidence from available test results to show a dependence of the absorption coefficients on potato variety, but the absorption coefficients at 10°C were lower than that at 4°C. The derived absorption coefficients of vapour CIPC by stored potatoes are 12.64 at 4°C and 7.89 at 10°C. These coefficients were used for the modelled results presented in this report unless specifically stated otherwise.

(5) The models have been validated against the results of pipe tests carried out by Glasgow University & Sutton Bridge Experimental Unit. The models gave predicted distribution patterns that showed the same trends as in the measured data. However, the predictions are generally lower than the measurements from the first test (i.e. Test A), but are in better agreement with the measurements from the repeated tests (i.e. Test B).

(6) Predictions have been made for CIPC vapour applications in a 12-tonne experimental store using a hot source (i.e. CIPC vapour is generated at high temperatures). The predicted vapour CIPC concentrations around the releasing point were higher than the saturation concentration, and so CIPC particles or solid deposits maybe formed during practical applications.

(7) The predicted CIPC absorptions in the store were more uniform when compared with the predicted deposits using conventional hot fog in a similar store (i.e. Y. Xu and D. Burfoot, 2000).

(8) The predictions for the 12-tonne experimental store could be much higher than measurements because the absorption of vapour CIPC by store walls & floor and by potato boxes are either not included or have been under-estimated in the models. Further adjustments to the models are needed to consider these undesirable CIPC losses (i.e. any CIPC absorption not on potatoes in the store) against measured values.

(9) The models are still to be tested against measurements from full-scale commercial potato stores.

CONTENTS

1 Introduction

Chlorpropham (CIPC) sprout suppressant is critical to the success of the UK potato industry. The use of the compound in Europe is being reviewed and could result in stricter control over its use. Currently, applications of CIPC are made as hot fog, a technique that usually results in variable distributions of the chemical and the quantity of the chemical required to achieve a good sprout control is relatively large. Stricter control of CIPC use may be introduced and could limit the number of applications of the chemical. This could subsequently compromise sprout control if the chemical is still going to be applied in the same as the current practice.

The use of vapour treatments or very small particles in a fogging treatment (particle diameters around 1 µm) gives the potential for improving the uniformity of CIPC treatments. Such approaches will only be effective if sufficient CIPC can be released into a store, air flow within the store can be managed to encourage effective dispersion of the released CIPC and the CIPC level can be maintained to the required level. This project aimed to assess the concept of sprout control using vapour and/or small particles of CIPC in stores and develop knowledge and data that are then used to create or adapt models to predict CIPC distributions. Validation of these models will enable them to be used to improve the application of CIPC and for this use to be regulated more closely.

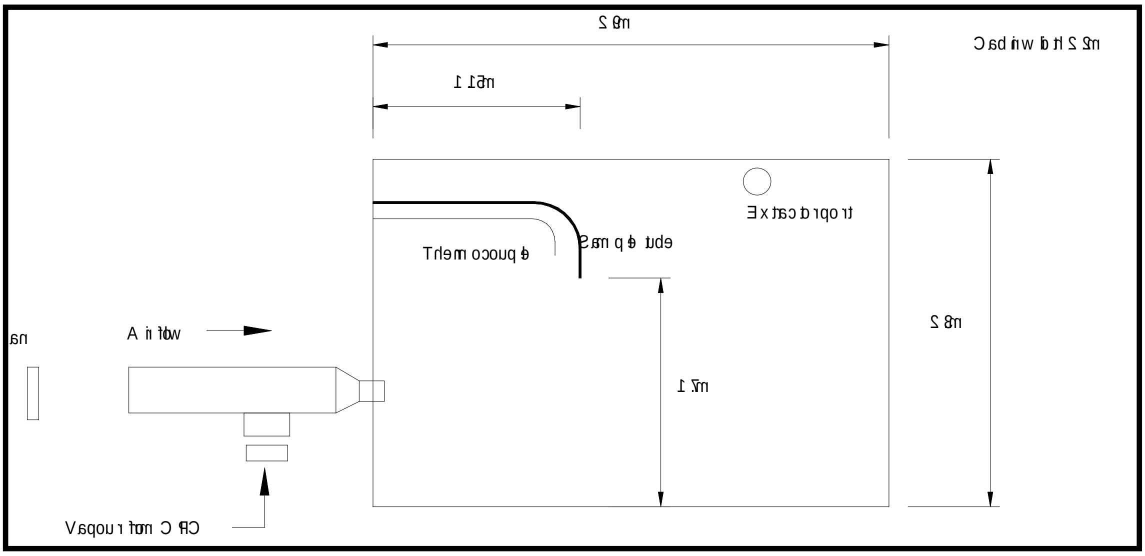
2. Preliminary experiments to explore the concept of using vapours and develop appropriate sources

The concept of using CIPC vapour to control sprouting in potato stores was initially examined by generating a vapour that was introduced into an air volume that in turn was monitored to track the formation of airborne particles. The form of the apparatus is shown in Figure 1. A source of solid CIPC formulation was placed on a hot plate mounted beneath a duct that was fully insulated. The duct was connected to a metal shipping container that had been lined with stainless steel sheet to give a smooth internal surface. Air was blown into the duct at a low velocity (circa 2.0 m/s). Conditions within the container were monitored by:

- measuring air temperature in the centre of the container; and
- drawing samples of air through a sample analyser measuring particle size and airborne concentrations in the different size fractions.

The container was vented to atmosphere via an extractor pipe that was connected to the back of the container at a high level and through which air could flow to enable vapour/particle laden air to enter the container. During the experiment, the generation and movement of vapour was also visualised by lighting the insulated duct.

Figure 1. Experimental layout for the initial experiments.



Two initial experiments were conducted and typical results are shown in Figure2. In the example run shown in Figure 2, the apparatus was operated at a steady state for approximately 45 minutes before the temperature of the CIPC was increased to increase the rate of vapour production. During the initial phase of the experiment vapour could be seen entering the test chamber but at a relatively slow rate. Increasing the temperature visually increased the rate of vapour production as expected. The result shown in Figure 2 indicates that the introduction of the vapour at the initial rate gave some formation of small airborne particles. However, the airborne concentration of these did not increase with time indicating that much of the CIPC material being introduced to the chamber was remaining as vapour. Increasing the temperature and hence the rate of vapour entry into the chamber did increase the concentration of particles suggesting that vapour was sublimating to form airborne particles. The temperature in the chamber for these two initial runs was in the range 10 to 16 ^{0}C although in subsequent runs conducted in warmer weathe, temperatures in the chamber exceeded 30 ^{0}C.

Experience gained from these initial experiments suggested that the concept of using a vapour source for treating a full-scale potato store was worthy of further investigation. Future experiments would need a vapour source with a known characteristic that:

- could have an output matched to the air volume to be treated;
- that would be stable over time;
- have a predictable emission for a given geometry of system;
- keep CIPC temperatures relatively low (<150 ^{0}C) so as to avoid chemical breakdown of the CIPC;
- preferably contain the CIPC in a non-metallic container also to minimise the risk of chemical breakdown.

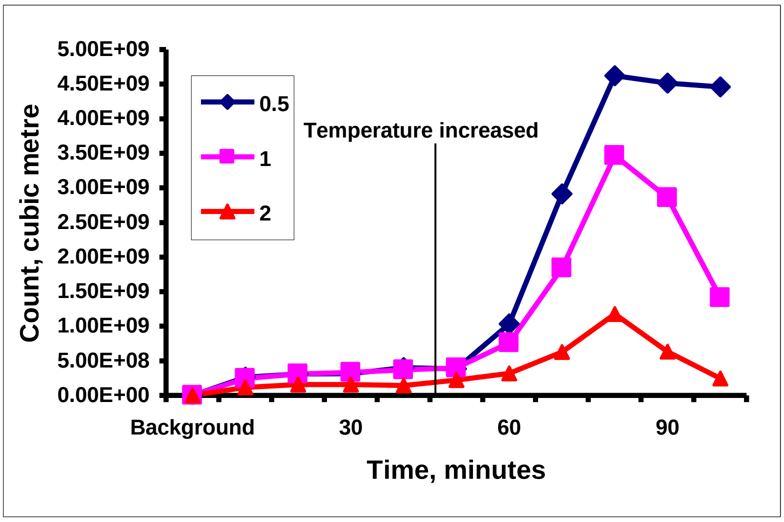


Figure 2(a). Particle sizes of between 0.5 and 2.0 µm measured in the chamber during initial experiments

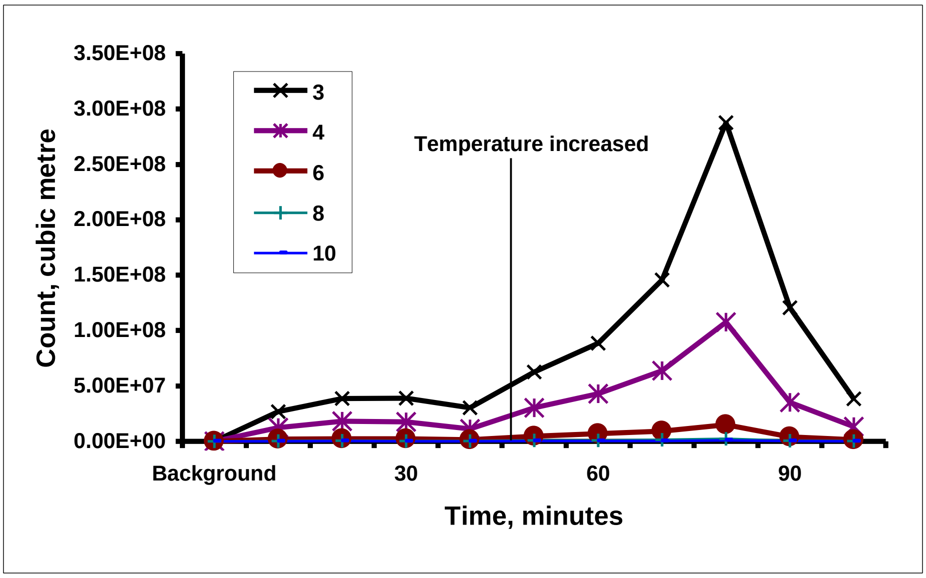


Figure 2(b). Particle sizes of between 3.0 and 10.0 µm measured in the chamber during initial experiments

An apparatus was devised in which a sample of CIPC was contained in a glass tube mounted in an oil bath. The oil bath was then positioned on a hot plate such that the temperature of the molten CIUPC could be controlled and measured directly. This arrangement was then calibrated to give a measured vapour release rate by recording the loss in weight over a three hour period for CIPC temperatures of between 130 and 160 ^{0}C. Results of the calibration experiments showed that for a given tube geometry, this heated source had a stable characteristic (see Figure 3) and a predictable release rate.

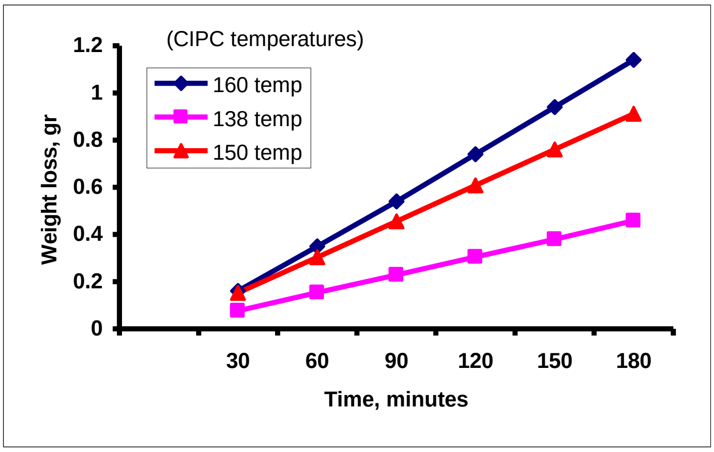


Figure 3. Loss rate of CIPC from a glass tube mounted in an oil bath

This arrangement was then used in two further experiments with the monitored chamber (Figure 1) with a CIPC release rate matched to the size of the chamber. These experiments monitored both the airborne particle size distribution in the chamber and also used sampling systems to monitor airborne vapour concentrations with the aim of accounting for all of the CIPC released. Examples of the monitored size distributions are summarised in Figure 4. The data plotted has been corrected to account for background airborne particle counts taken immediately before the run. For one of the runs (shown in Figure 4(b)), the background levels were high because dust had been disturbed with the chamber by the installation of suction sampling tubes for vapour analysis. In another run, high background levels were monitored because an air compressor operating in the same building was found to be emitting airborne oil droplets of 0.5 μm diameter.

The results from both sets of runs confirmed that vapour could be released into the chamber at low concentrations without forming particles when in contact with cold air. Attempts to monitor the amount of CIPC introduced as vapour were not successful because the walls of the chamber had become contaminated with CIPC during the first series of experiments and tended to act as a secondary source during the later work.

It was recognised that the use of a heated source would need the vapour to be released in to a fast moving air flow to prevent high vapour concentrations meeting cooler air and sublimating to form particles. A unit was designed and constructed for use in experiments at Sutton Bridge Experimental Unit (Figure 5) in which an oil filled flask was mounted together with an electrical heating element and temperature sensor (platinum resistance thermometer) in to an insulated tube. The mains powered heating element and electrical thermometer were connected to a commercial design of process control unit such that the temperature of the oil, and hence of the CIPC could be controlled to pre-set values.

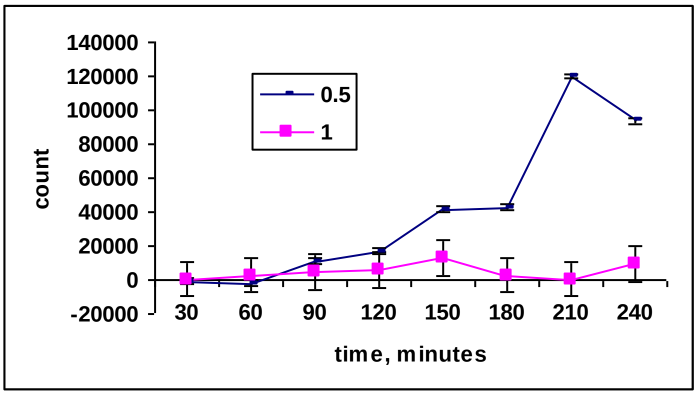


Figure 4(a). Measured airborne concentrations in the chamber treated with a controlled vapour source – Run 3

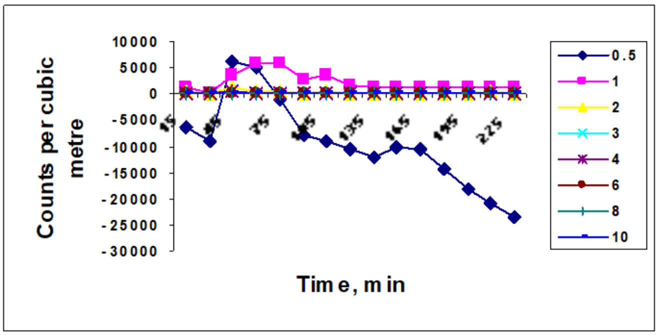


Figure 4(b). Measured airborne concentrations in the chamber treated with a controlled vapour source – Run 4

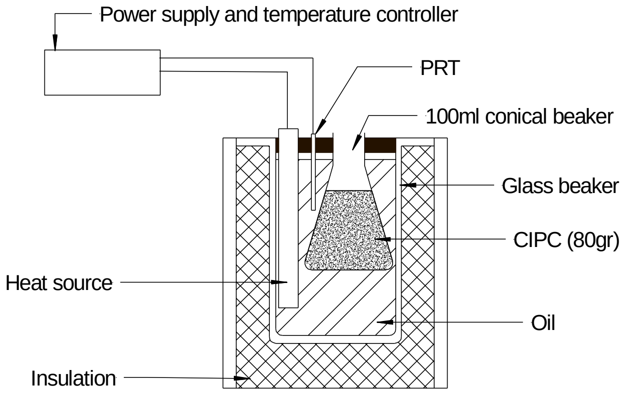


Figure 5. Controlled hot source

The unit shown in Figure 5 was then used in experiments with experimental 12 tonne stores at Sutton Bridge – see Section 6 of this report.

3 The modelling approach

3.1 The model

The capabilities of computational modelling in potato storage have been demonstrated by previous work in an experimental store (Y. Xu and D. Burfoot, 2000) and in a commercial potato store (Y. Xu, D. Burfoot & P. Huxtable, 2002). However, these models need to be extended and validated for the applications of CIPC vapour.

The models for the application of vapour CIPC have to include three essential components to simulate CIPC applications in potato stores, i.e. CIPC releasing into air, transportation by air movements and absorption by potatoes, as shown in Figure 6. The models for CIPC release and absorption are based on Henry's law and supported by experiments to provide the required parameters. The transfer process can be simulated by solving the Navier-Stokes equations governing the movement of airflow and vapour CIPC using Computational Fluid Dynamics (CFD).

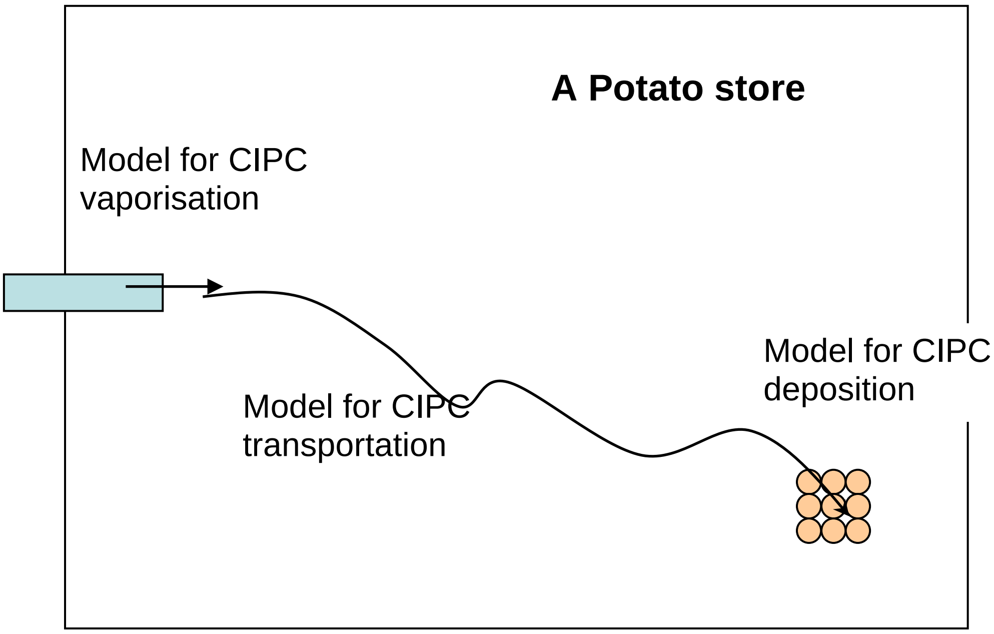


Figure 6. Components of the computer model for the application of vapour CIPC in potato stores

Figure 7 illustrates the evaporation of vapour CIPC from the solid phase and the absorption of vapour CIPC by potatoes. Based on Henry's law, the rate of evaporation can be calculated as:

$$q_1 = k_1(P_{vp} - P^{'}) \qquad (1)$$

where k_1 is a partitioning constant which is dependent on local air temperature and air velocity, P_{vp} is CIPC vapour pressure on the solid phase and P' is the local partial pressure of CIPC vapour in the air stream. Both P_{vp} and P' are temperature dependent. The total amount of vapour CIPC evaporated during a period is the product of the rate of evaporation and surface area of the solid CIPC and time.

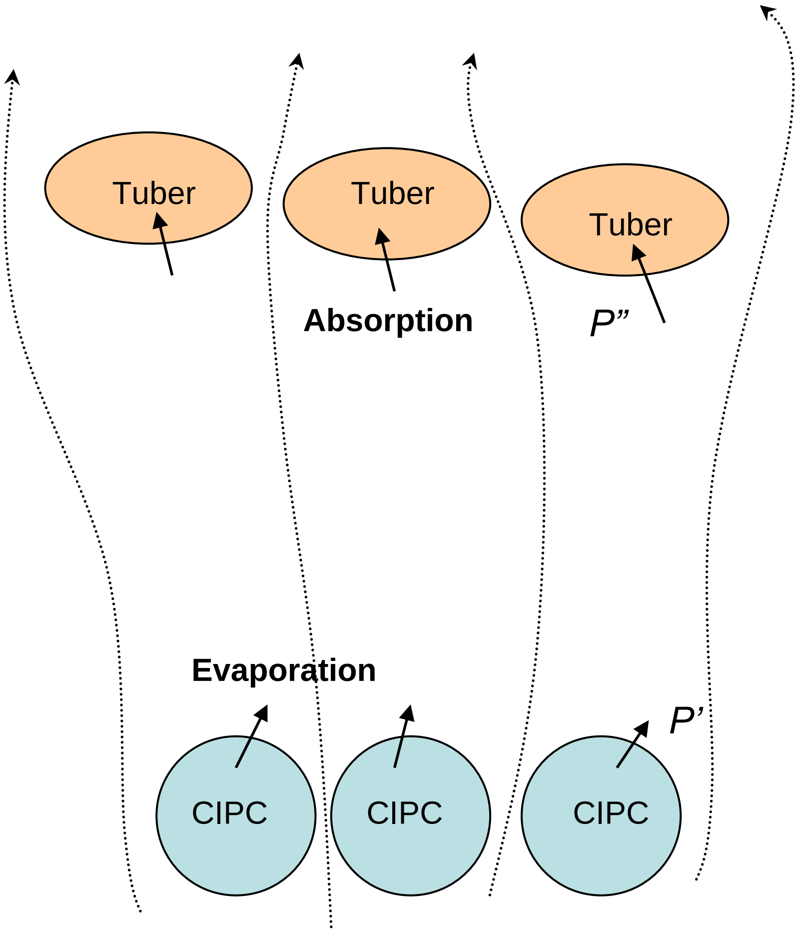


Figure 7: Illustrations of the evaporation and absorption processes

The absorption rate of vapour CIPC by potatoes can be expressed as:

$$q_2 = k_2(C_s^{equ} - k_3 C_s) \qquad (2)$$

where k_2 is the absorption rate which is temperature dependent, k_3 equals 1 for an exponential absorption model or 0 for a linear absorption model. These two absorption models were assessed in this study as given later in Section 5 and the most suitable model was selected. C_s is the concentration of absorbed CIPC on tuber surfaces and C_s^{equ} is the equilibrium CIPC concentration over the tuber surfaces which is related to the local partial pressure of CIPC vapour P'' as:

$$C_s^{equ} = C_{sol} P'' \qquad (3)$$

where C_{sol} is the solubility of CIPC vapour on potato surfaces and P'' is the local partial pressure of CIPC vapour around the potatoes.

The models for evaporation and absorption were linked through the transportation equation for vapour CIPC, which was solved together with the equations for air movements through the computational model developed at SRI for potato storage. So *P"* and *P'* in equations 1 & 3 are related precisely according to the actual ventilation system and the setup of each potato store, the temporal and spatial variations of CIPC deposition are predicted and the application of vapour CIPC can be optimised. These models were validated step-by-step against data from controlled experiments in this study and the results were given in this report.

3.2 Input data for the model

- Data required by the evaporation model (i.e. Equation 1) are the partitioning constant k_1 and CIPC vapour pressure P_{vp}. This model is suitable for the evaporation of CIPC from the solid phase. A different model would be needed if the vapour CIPC is generated using other methods, such as the hot source described later in Section 5.
- Data required by the absorption model are the absorption constant k_2 and the solubility of CIPC vapour on potato surfaces if the exponential absorption model is used. These parameters were derived from tests carried out at experimental stores at SBEU as given in Section 4.

3.3 Validating the model

- Pipe tests. Vapour CIPC was passed through potatoes packed inside a straight pipe. Measurements were taken for CIPC concentrations in air and the deposits on potato samples. These one-dimensional tests were conducted under well-controlled conditions and enabled the validation of the computer models developed efficiently. The accuracy and the validity of the models were assessed against the results from the pipe tests.
- Tests in experimental potato stores: These small-scale three-dimensional tests were conducted in the 12-tonne experimental stores at SBEU. The controllability of these tests is good and the computational models for these stores are potentially simple and accurate. It normally requires a huge computing power and resources to obtain accurate simulations of CIPC applications in these test cases and commercial stores for a moderate test period. Simplified modelling strategies were developed and validate against the test results from these experimental stores. Other factors could be investigated using the results of these tests include the absorption of vapour CIPC by the store walls and potato boxes and CIPC introduction positions and methods. The strategies for the application of vapour CIPC in commercial stores can also be initiated and tested in small scales using the test results.
- Measurements in a commercial potato store. These measurements will be used to test the models further and then the model can be used to establish strategies for optimised CIPC applications in a range of stores. No measurement and prediction have been done in this area at the time of preparing this report.

4 Deriving the absorption coefficients

4.1 The methods

The absorption of vapour CIPC could be modelled in two ways, i.e. linear or exponential absorptions. The linear model assumes that the absorption is linearly related to the local CIPC vapour pressure and is not affected by CIPC deposit on the tuber surfaces. In the exponential model, the absorption will slow down gradually as the increase of CIPC deposition on the tuber surfaces. Measurements of CIPC absorption by potatoes were fitted to the forms of these two models to obtain the coefficients required. Then both models were validated against the results of the pipe tests and the model that produced better predictions was selected for the modelling study of the small-scale experimental stores and the commercial store.

4.1.1 Linear absorption model

The linear absorption can be expressed as:

$$\Delta m = k_1 P_{vp} S \Delta t \quad (4)$$

where m is the mass of absorbed CIPC, k_1 is the absorption coefficient, P_{vp} is the local CIPC vapour pressure, S is the tuber surface area, t is time and Δt is the time step.

Assuming constant local vapour pressure, the total absorption is:

$$m = k_1 P_{vp} St + C_0 \quad (5)$$

Converting the absorption to the unit of the measured CIPC residuals (i.e. mg CIPC / kg potato), Equation 5 becomes:

$$C = \frac{m}{F} = \frac{k_1 P_{vp} St}{F} + \frac{C_0}{F} \quad (6)$$

where C the surface CIPC concentration of the potatoes and F is a conversion factor.

Fitting the experimental data to the same format as Equation 6, i.e.

$$C = at + b \quad (7)$$

Therefore

$$a = k_1 P_{vp} S / F \quad (8)$$

The absorption coefficient is:

$$k_1 = \frac{aF}{P_{vp} S} \quad (9)$$

<u>Observations on these parameters:</u>

- ***a*** is dependent on CIPC vapour pressure, temperature, potato size, type and the ways potatoes were exposed (i.e. single layer or boxes).
- ***k₁***.should be only dependent on temperature and maybe potato type, and is the factor to be derived from the measurements.
- *b* represents the initial CIPC residuals on potatoes and it should be near zero if the potatoes are CIPC free before the tests.

4.1.2 Exponential absorption model

The exponential absorption can be expressed as:

$$\Delta m = k_1 (C_{sol} P_{vp} - C) S \Delta t \qquad (10)$$

Where C_{sol} is the solubility of vapour CIPC on potatoes and C is the absorbed CIPC concentration on potatoes.

The total absorption is

$$m = C_{sol} P_{vp} - (C_{sol} P_{vp} - C_0) e^{-k_1 St} \qquad (11)$$

and

$$C = \frac{C_{sol} P_{vp}}{F} - \frac{(C_{sol} P_{vp} - C_0) e^{-k_1 St}}{F} \qquad (12)$$

Fitting the experimental data to the same format as Equation 12, i.e.

$$C = a - be^{-ct} \qquad (13)$$

Therefore

$$a = C_{sol} P_{vp} / F \qquad (14)$$

$$b = (C_{sol} P_{vp} - C_o) / F \qquad (15)$$

$$c = k_1 S \qquad (16)$$

The parametrs required by the expontial model are:

$$k_1 = c / S \qquad (17)$$

$$C_{sol} = aF / P_{vp} \qquad (18)$$

<u>Observations on the parameters:</u>

- ***a, b & c*** are dependent on CIPC vapour pressure, temperature, potato size, type and the ways potatoes were exposed (i.e. single layer or boxes).
- ***k***.& ***C_{sol}*** should be only dependent on temperature and maybe potato type, are derived from the measurements.

- For absorption tests carried out on new potatoes or on potatoes without initial CIPC residual, C_0 is zero and parameters *a* and *b* are equal.

4.2 Deriving the coefficients

The experimental data used to derive the coefficients required came from the contamination tests carried out by SBEU & Glasgow University. The study was set up to investigate the effect of CIPC absorption by air temperature, crop loading (i.e. the amount of crop in the store) and cultivar. The only source of vapour CIPC in the store was fabric of the test stores (e.g. floor, walls & potato boxes) contaminated as a result of previous applications.

The tests stores were run under the following conditions:

Store 33:	4ºC, 95% RH. One tonne of each of Saturna, Russet Burbank and Maris Piper in one-tonne boxes.
Store 34:	4ºC 95% RH. 10kg of each of Saturna, Russet Burbank and Maris Piper in trays placed in empty potato boxes.
Store 35:	10ºC, 95% RH. One tonne of each of Saturna, Russet Burbank and Maris Piper in one-tonne boxes.
Store 36:	10ºC, 95% RH. 10kg of each of Saturna, Russet Burbank and Maris Piper in trays placed in empty potato boxes.

In each store, three one-tonne boxes were laid out on the floor and each box was full in the case of stores containing 3 tonnes of crop. In the other stores, three 10kg trays were placed inside empty boxes, and 10kg of crop was divided among the three in a single layer.

Three tubers were removed from each box or tray on each sampling occasion to get an idea of variability. Tubers were collected at Day 0 (before study began) 1, 4, 7, 14, 28 and 35 of a five-week storage period.

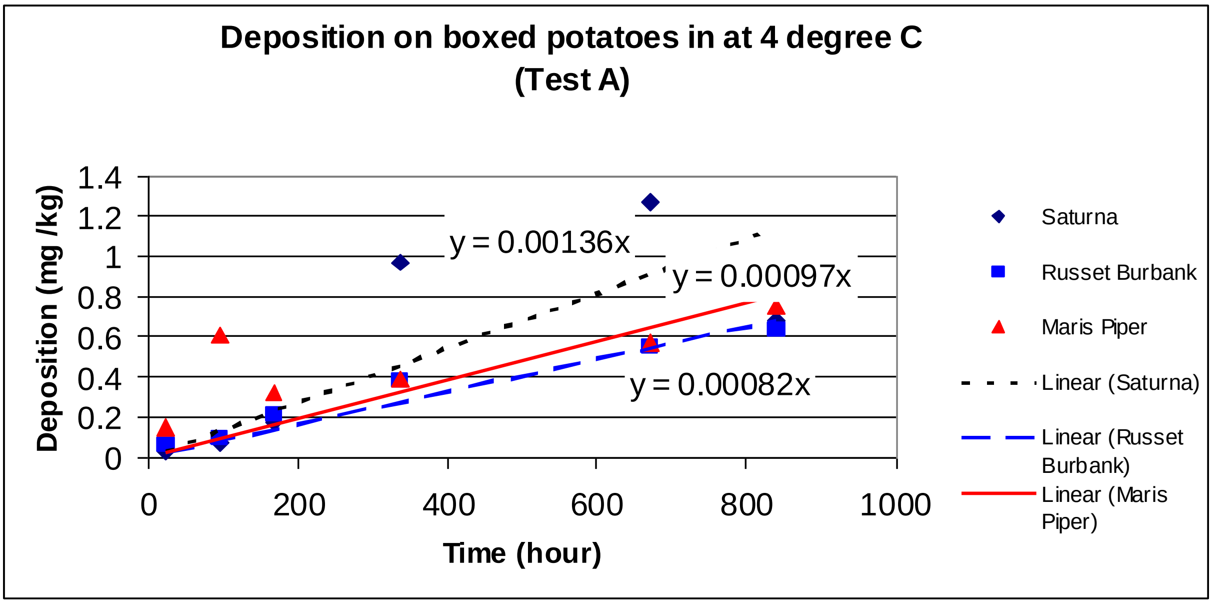
The tests were repeated once to check their repeatability and they are quoted as Test A (i.e. the first set of tests) and Test B (i.e. the repeated tests) in this report.

4.3 Analysing the test results

The following assumptions were made while analysing the measurements:

1. CIPC residuals on all sample potatoes are zero at the start of the tests (e.g. the fitted curve for each test case passes through the origin, i.e. zeroed as mentioned in the figures).
2. All sample potatoes have similar sizes.
3. The conditions (both physical and physiological conditions) of sample potatoes of the same cultivar are similar in both sets of tests.
4. Tests A & B were conducted under very similar controlled conditions, apart from the store vapour CIPC concentrations that were measured and were taken into consideration in the analysis.
5. Only 75% of the surface areas of the top layer potatoes in boxes are freely exposed to vapour CIPC (e.g. the top half is exposed fully and only half of the lower half is exposed for each top layer potato). This assumption makes the results of boxed potatoes and the potatoes in trays under similar test conditions comparable.

Figure 8 shows the linear regression of the test results to derive the parameters in Equation 7 for the tests of Test A at 4 ^{o}C. The straight lines were forced to pass the origin by assuming no initial CIPC residuals on the potatoes. These parameters were then converted to the absorption coefficient using Equation 10. The derived absorption coefficients are summarised in Table 1 and shown in figures 9 -12.



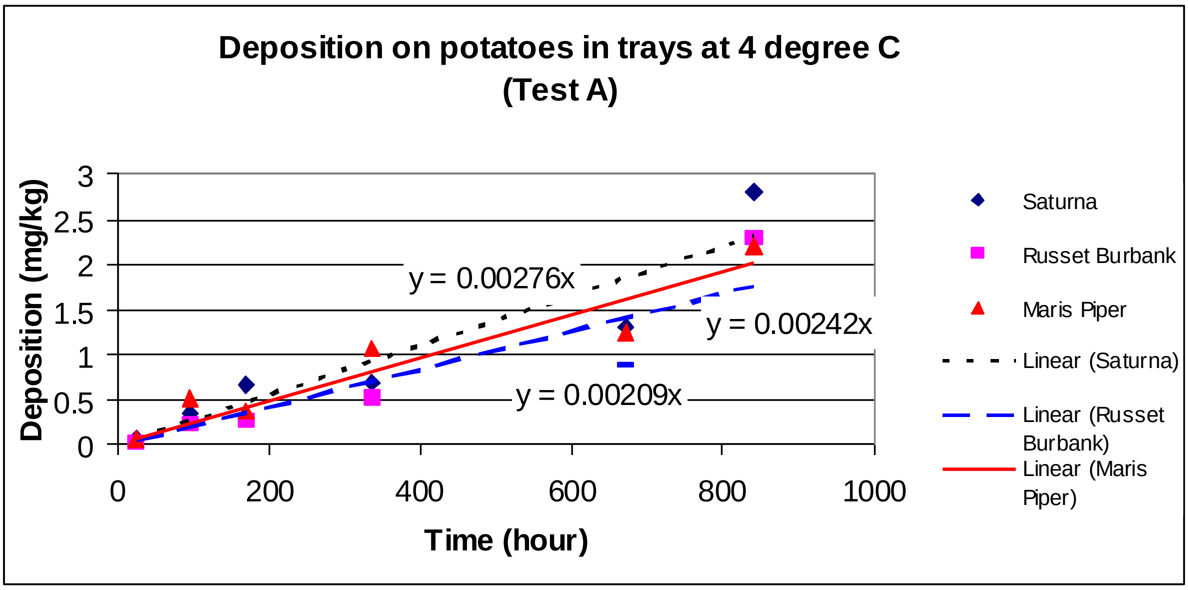


Figure 8: Linear regression of the measurements for the parameters required by the linear absorption model

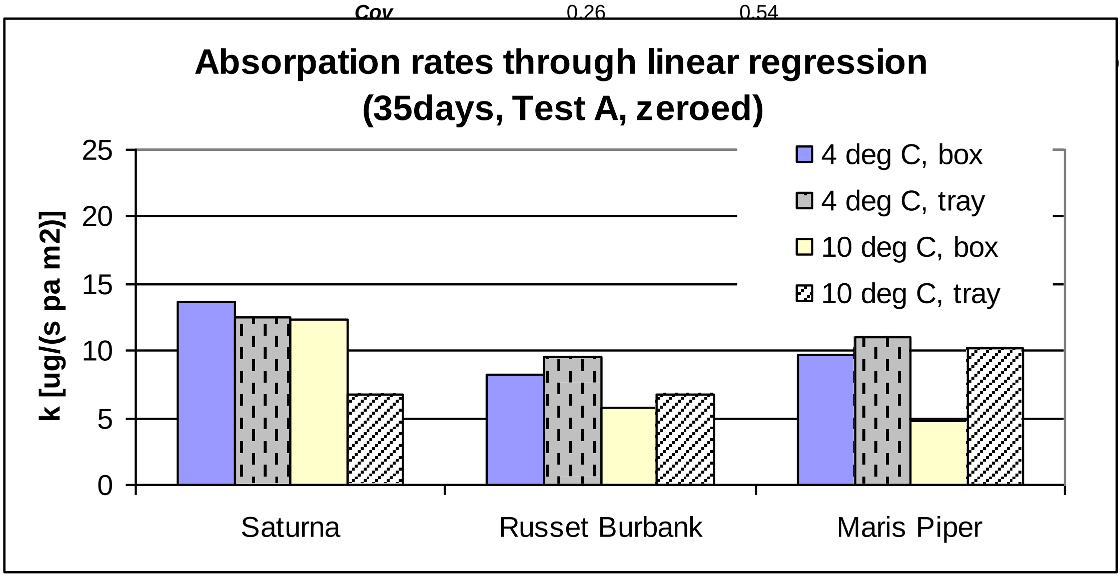
Table 1

Figure 9. The derived absorption coefficients from the results of test A

Comparison of the results of tests A & B

	4°C box	4°C tray	10°C box	10°C tray	10°C Avg	Diff of A&B %	4°C Avg	Diff of A&B %	All Avg	Diff of A&B %			Diff of A&B %
Test A													
Saturna	13.63	12.55	12.27	6.79	9.53		13.09		11.31		**4°C average of all varaities**	10.77	
Russet Burbank	8.22	9.51	5.80	6.79	6.29		8.86		7.58		**10°C average of all varaities**	7.77	
Maris Piper	9.72	11.01	4.71	10.23	7.47		10.36		8.92		**Average of all varaities**	9.27	
Test B													
Saturna	20.46	15.28	5.60	10.65	8.12	***-15***	17.87	**37**	13.00	***15***	**4°C average of all varaities**	14.50	***35***
Russet Burbank	11.62	17.17	15.96	7.92	11.94	***90***	14.39	**62**	13.17	***74***	**10°C average of all varaities**	8.01	***3***
Maris piper	13.53	8.97	2.97	4.99	3.98	***-47***	11.25	**9**	7.62	***-15***	**Average of all varaities**	11.26	***21***

		4 °C	10 °C	Reduction due to temperature
Test A	***mean***	10.77	7.77	**-0.28**
	sdv	1.85	2.63	
	cov	0.17	0.34	
Test B	***mean***	14.50	8.01	**-0.45**
	sdv	3.72	4.29	
	Cov	0.26	0.54	
				.38



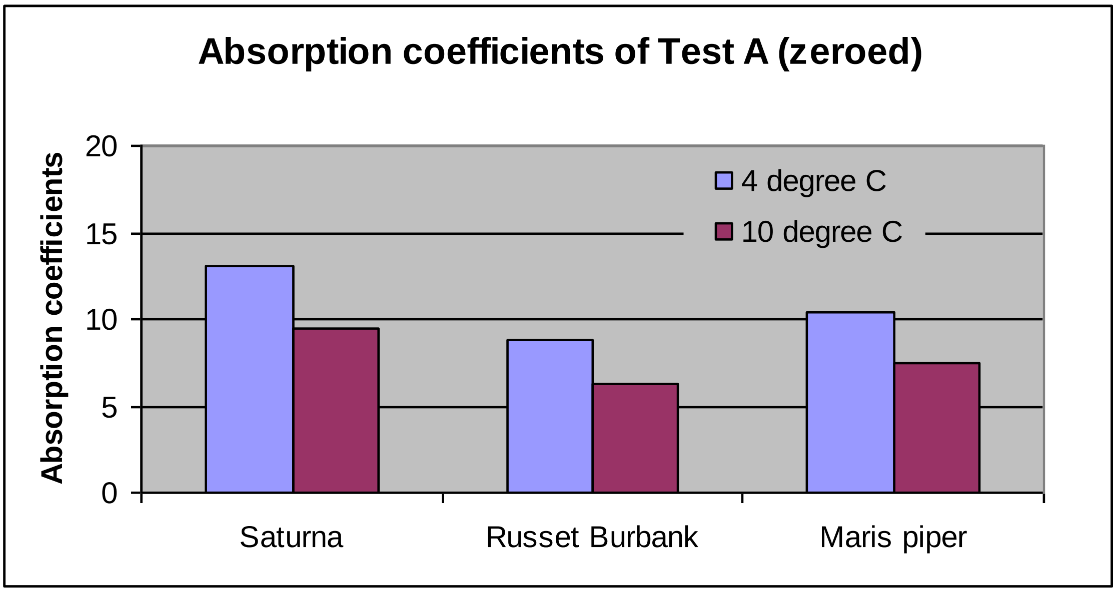


Figure 10. The change of absorption coefficients with temperature and potato variety (test A)

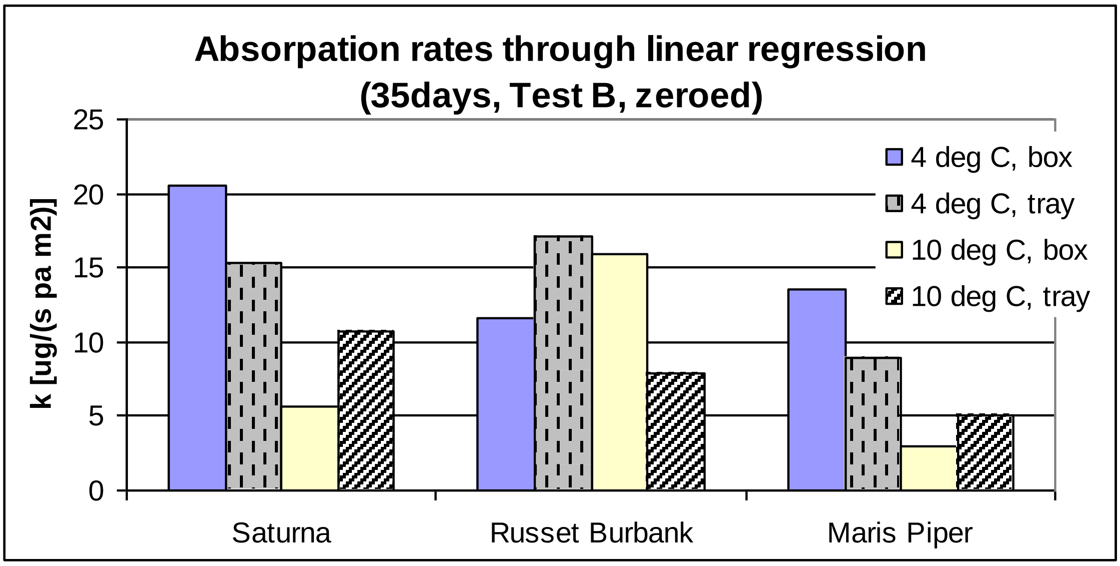


Figure 11. The derived absorption coefficients from the results of test B

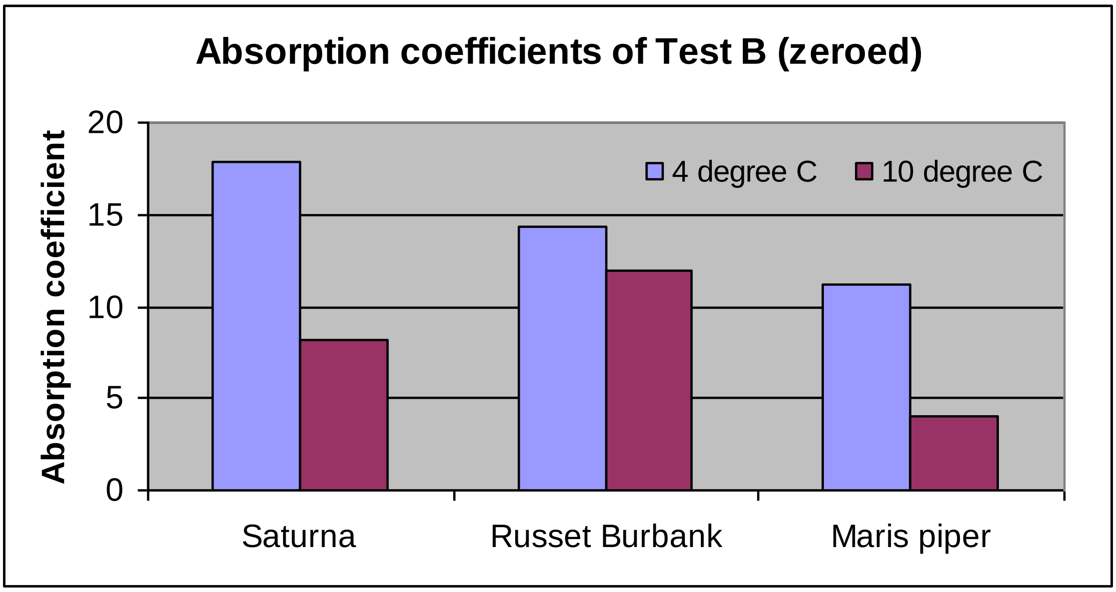


Figure 12. The change of absorption coefficients with temperature and potato variety (test B)

Figures 13 –14 show the parameters derived for the exponential absorption model from the results of test A. In the results to be given in Section 5 in this report, the exponential absorption model was shown to be no better than the linear model, so the linear absorption function was selected for the modelling of potato stores due to its simplicity. Therefore, only the absorption coefficients for the linear model were analysed in details in this study and in the conclusions given below.

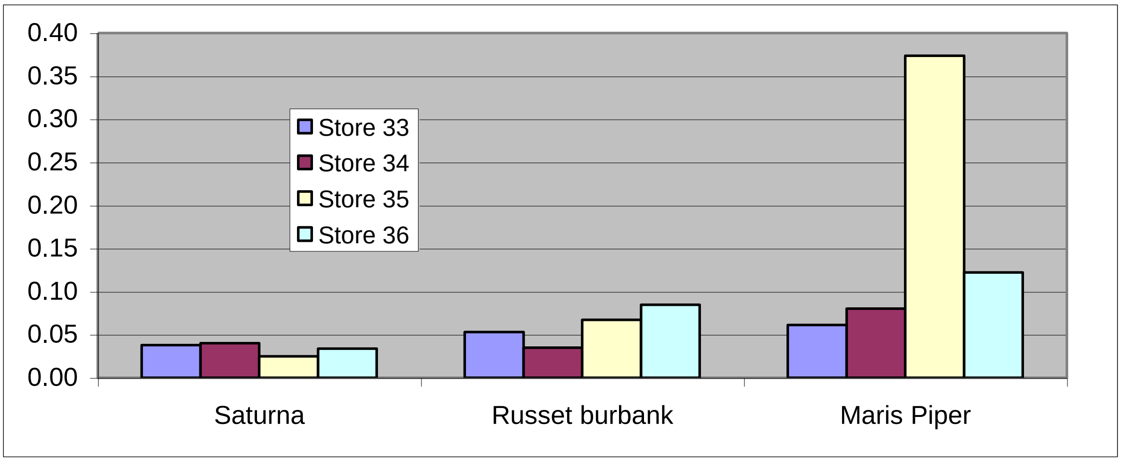


Figure 13. The derived absorption coefficients for the exponential model from the results of Test A

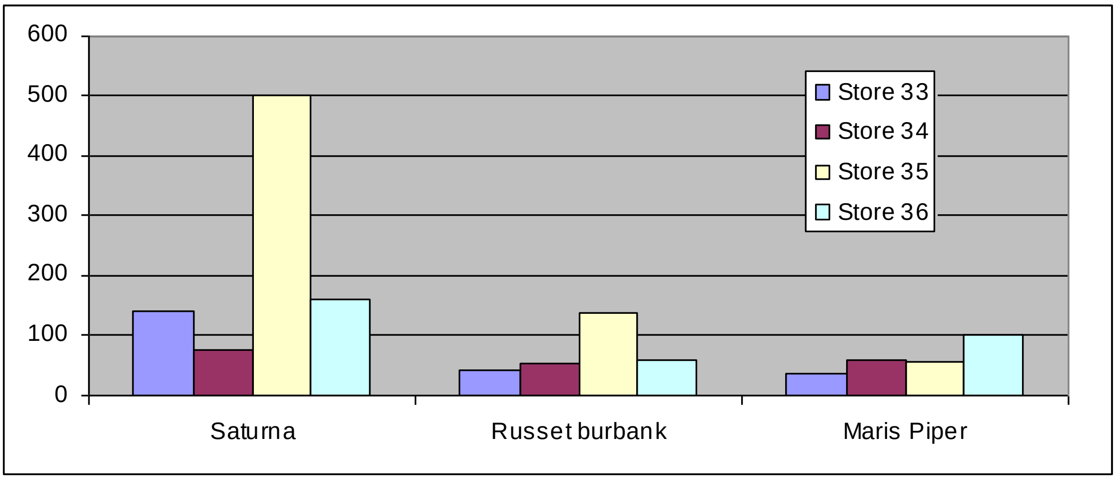


Figure 14. The derived solubility of vapour CIPC on potatoes for the exponential model from the results of Test A

4.4 Conclusions

1. The absorption coefficients of Test B are generally higher than that of Test A, which are 35% higher at 4°C and 3% higher at 10°C.

2. The standard deviations & the coefficients of variation (Cov) of the absorption coefficients are also higher in Test B. The Covs of Test A are 0.17 & 0.35 at 4°C and 10°C, and they are 0.26 & 0.55 in Test B.

3. The two tests are thought to be consistent to each other reasonably, thought it is difficult to quantify the achievable and acceptable level of consistency for this kind of tests.

4. No clear evidence to show the dependence of the absorption coefficients on potato variety.

5. In both tests and for each variety, the absorption coefficients at 10°C are lower than that at 4°C. The difference of the averaged absorption coefficient of all varieties at the two tested temperatures is 28 % in Test A between the two tested temperatures and is 45% in Test B.

6. The average value of the absorption coefficients of all varieties of both tests at a particular temperature is to be used as the absorption coefficient of all potato varieties at that temperature in future modelling work of this project. The absorption coefficients of vapour CIPC by stored potatoes are 12.64 at 4°C and 7.89 at 10°C. These are the coefficients to be used for modelling presented below unless it is specially mentioned.

5 Testing the model: one-dimensional tube tests

Simplifications and assumptions were made to develop the models for the application of vapour CIPC. Before these models could be applied confidently to formulate strategies for applying vapour CIPC in commercial potato stores, they have to be validated against well-controlled tests. The validation should establish the capabilities of the model, such as their strength and weakness, the prediction accuracy, the scope they can be applied and the ways they are going to be used.

Figure 15 shows the pipe experiments carried out at Sutton Bridge for this purpose. In each test, a vertical pipe, 1.5m long with an internal diameter of 300mm, was located in an experimental store that was contaminated by CIPC applications in previous years. Each pipe contained potatoes of 1m depth (approx. 40 kg) and air was sucked through the packed potatoes by a fan placed over the upper end.

Figure 15. Pipe apparatus used at Sutton Bridge Experimental Unit.

Two sets of pipe tests were carried out, e.g. Test A conducted in November-December 2004 and Test B in April-May 2005. Each set has four tests having different air velocities drawn through the pipes. The test duration is 19 days for Test A and is 11 and 19 days for Test B. CIPC absorptions by potatoes were measured at six positions at 25mm (Layer 1 at the inlet), 75mm (Layer 2), 200mm, 300mm, 600mm & 900mm from the inlet.

In these tests, the sources of vapour CIPC were the walls & floors of the stores that were contaminated by CIPC applications in previous years, and the airborne CIPC concentrations were measured frequently during the tests as shown in Table 2 for Test A. The evaporated vapour CIPC was then drawn into the pipes at various speeds and absorbed by the packed potatoes. The air velocities passing through the pipe are given in Table 3.

Table 2: Measured vapour CIPC concentrations (µg/l) in test stores (Test A)

	Store 32	**Store 33**	**Store 34**
Day 1	0.174	0.115	0.015
Day 7	0.116	0.091	0.071

Day 17	0.087	---	0.091

Store 32 contained the slow flow and no flow pipes
Store 33 contained the medium flow pipe only
Store 34 contained the fast flow pipe only

Table 3: Air speeds through the pipes

Test cases	**First set tests (Test A)**	**Second set tests (Test B)**
High flow	0.44-0.48 m/s	NA
Medium flow	0.26-0.28 m/s	0.28-0.29 m/s
Low flow	0.05-0.09 m/s	0.06-0.07 m/s
Very low flow	NA	0.02-0.03 m/s
No flow	0.0	0.0

5.1 Validating the model against the earlier tests results (Test A)

In the model, the concentrations of vapour CIPC at the inlet of the pipe are assumed to be the room CIPC concentrations of the stores that were measured as shown in Table 2, and no attempt was made to estimate the CIPC evaporation rates from the store walls & floors. So the evaporation process was not actually included in the model and the validation here is only for the modelling components for CIPC convection and absorption as shown in Figure 6. The potatoes used for this test were Saturna and tests had been carried out to measure its absorption coefficient as given in Section 4. The absorption coefficient used is 9.8 as shown in Figure 9.

Figure 16 shows the measured CIPC absorptions and the trend lines of the four test cases of test A. High airflow through the pipe (i.e. a velocity of 0.44 - 0.48 m/s) has produced the highest CIPC absorption and the trend line is almost flat crossing the potato pack. When the flow is dropped to 0.05m/s, the absorption at the inlet is still as strong as in the high flow case, but it has gradually reduced towards the outlet. Therefore the gradients of CIPC absorption increase as the pipe flow decreases. When there is no flow through the pipe, only the potatoes next to both ends of the pack had meaningful absorption due to the diffusion process.

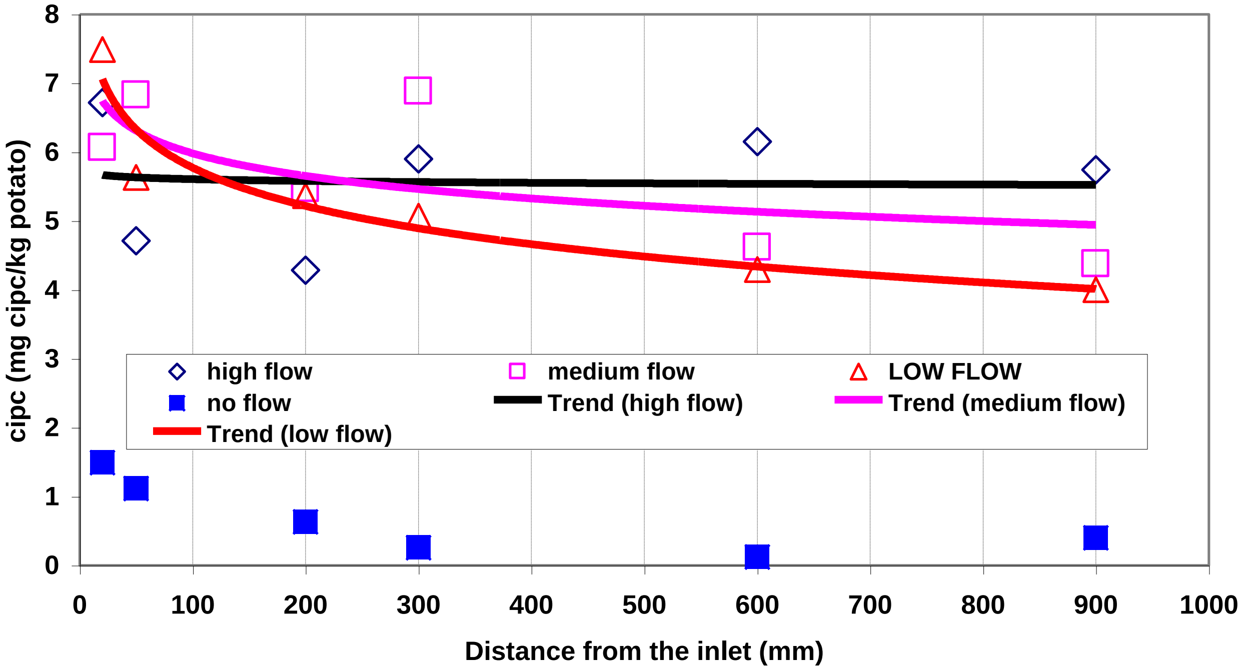


Figure 16. Measured CIPC absorption in the first pipe test.

Figure 17 shows the predicted CIPC absorption of Test A using the linear model. As measured, the absorption is very flow in ‘Medium flow’ case and the gradients of the absorption crossing the potato pack increase as the air velocity decreases. The model has performed as observed qualitatively. However, the very high absorption by the potatoes near to the inlet was not predicted by the model.

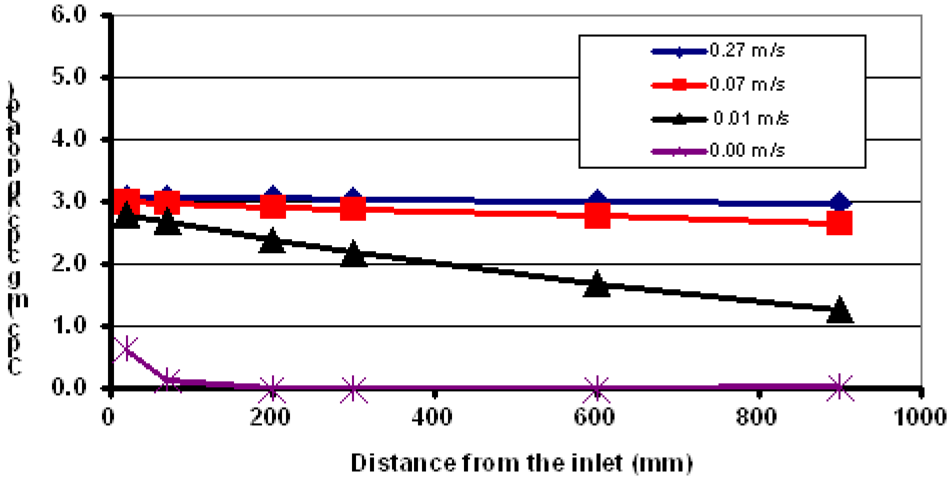


Figure 17. The predicted absorption for pipe test A
(the linear model)

Figure 18 shows the comparison of the predicted CIPC absorptions using the linear and the exponential absorption models for the 19-day period of test A. As expected, the predicted absorptions by the exponential model are lower at the inlet and trend lines are more flat. However, the differences between the predictions by the two models are quite small. Because of these small differences, the linear absorption model was selected for subsequent investigations because of its simplicity and only one parameter is required. Therefore only the predictions using the linear model are presented from here forward.

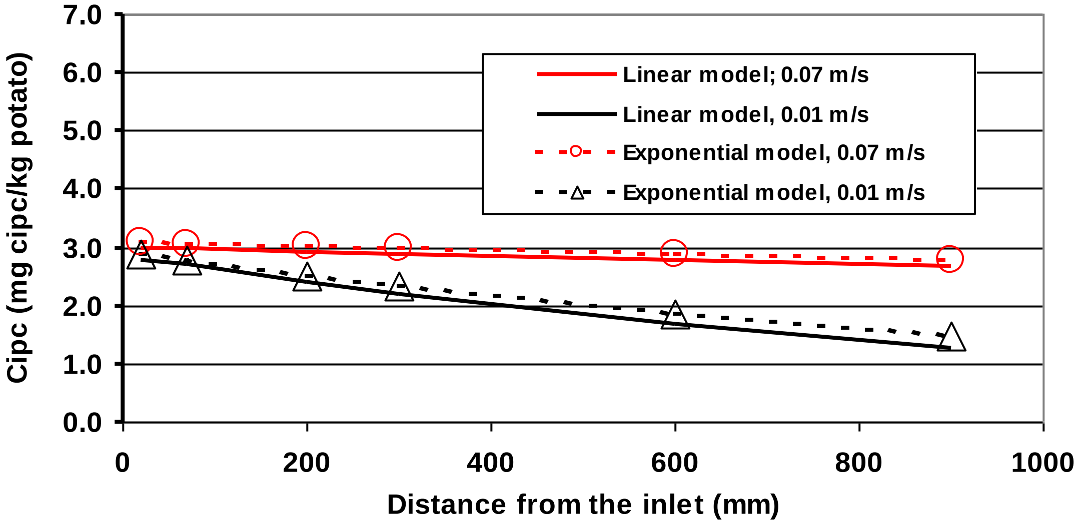


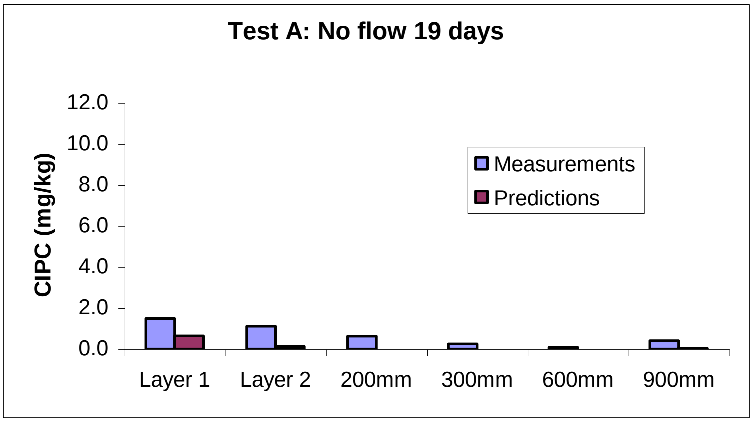
Figure 18. Comparing the predictions of the linear and exponential models

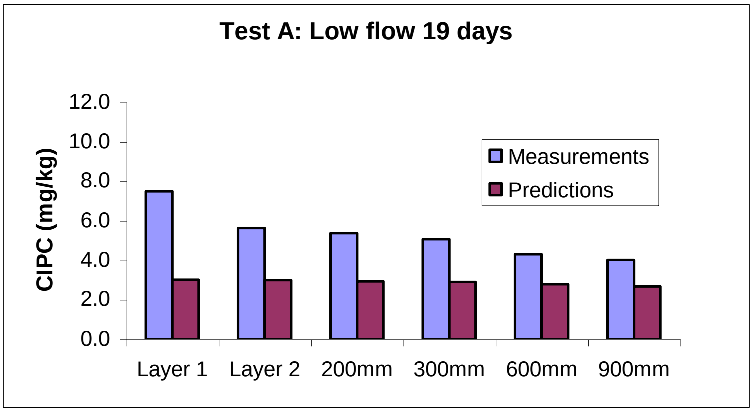
Figure 19 shows the comparison between the predicted and measured absorptions of Test A. The model has under-predicted the absorptions in all cases, particularly in the inlet area. The predicted values are only half of the measurements at the inlet. The agreement at the outlet areas is much better. Many factors could have contributed to the differences, including the measuring accuracies of the absorption coefficients and the flow rate, the assumption of uniform potato diameter, and it is difficult to quantify the contributions of these parameters to the differences. To illustrate the influence of these factors on the predicted absorption, Figure 20 shows the results of a sensitivity study with assumed absorption coefficient and flow rate. A 15% increase of the absorption coefficient and a drop of pipe velocity from 0.07 m/s to 0.056 m/s would have caused the prediction to improve. Figure 21 shows the effect of potato size on the predictions. When the potato diameter is reduced from 58mm to 50mm, the predicted absorptions get very close to the measurements. The diameter range of the potatoes used in the tests is between 40-70 mm, and the weight averaged diameter of all potatoes is 58mm. In the model, all potatoes are assumed to have a diameter of 58mm.

5.2 Validating the model against the repeated tests (Test B)

A repeat of the pipe experiment was carried out to check the repeatability of the tests and validate the predictions further. In test B, the case of ‘high flow’ was dropped because the flow is significantly faster than what would find in real potato stores, and a case of ‘Very very low flow’ was introduced. The measured velocity of the case of ‘Very low flow‘ is between 0.02-0.03 m/s as shown in Table 3.

In test B, the potatoes used are Sante, instead of Saturna used in test A, and the mean diameter of the potatoes is 50 mm. Because no test has been done to measure the absorption coefficient of Santa as shown in section 3. The absorption coefficient used in the model for test B is 7.89, as concluded in section 3.4 for all potato types.





Figures 22a & 22b show the comparison of the predictions against measurements in a 19-day period. Even though depositions are still under-predicted, the agreements are generally better in all cases compared with the predictions for Test A. For the case of ‘very low flow’, the predicted depositions are within the estimated range at all measurement positions. Compared with test A for Saturna in a 19-day period, the measured depositions have halved with the highest deposition around 3.5 mg /kg in this test, against 7.5 mg/kg in test A. Modelling results have shown that the reduction in potato size has made a large contribution to the reduction of measured absorptions.

Figures 23a & 23b show the comparison of the predictions against measurements for an 11-day period. The agreement of this test case is not as good as for the 19-day period and this maybe is due to the fact that the absorption coefficients used in the models were obtained from tests which had lasted up to 5 weeks and the coefficients derived should be more suitable for the 19-day period.

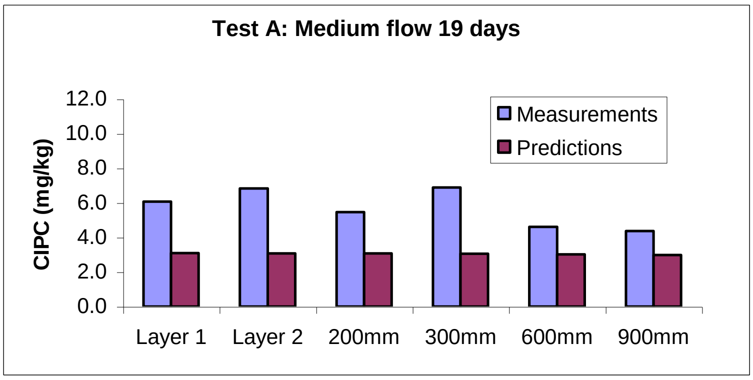


Figure 19. Comparing measured and predicted deposits (Test A)

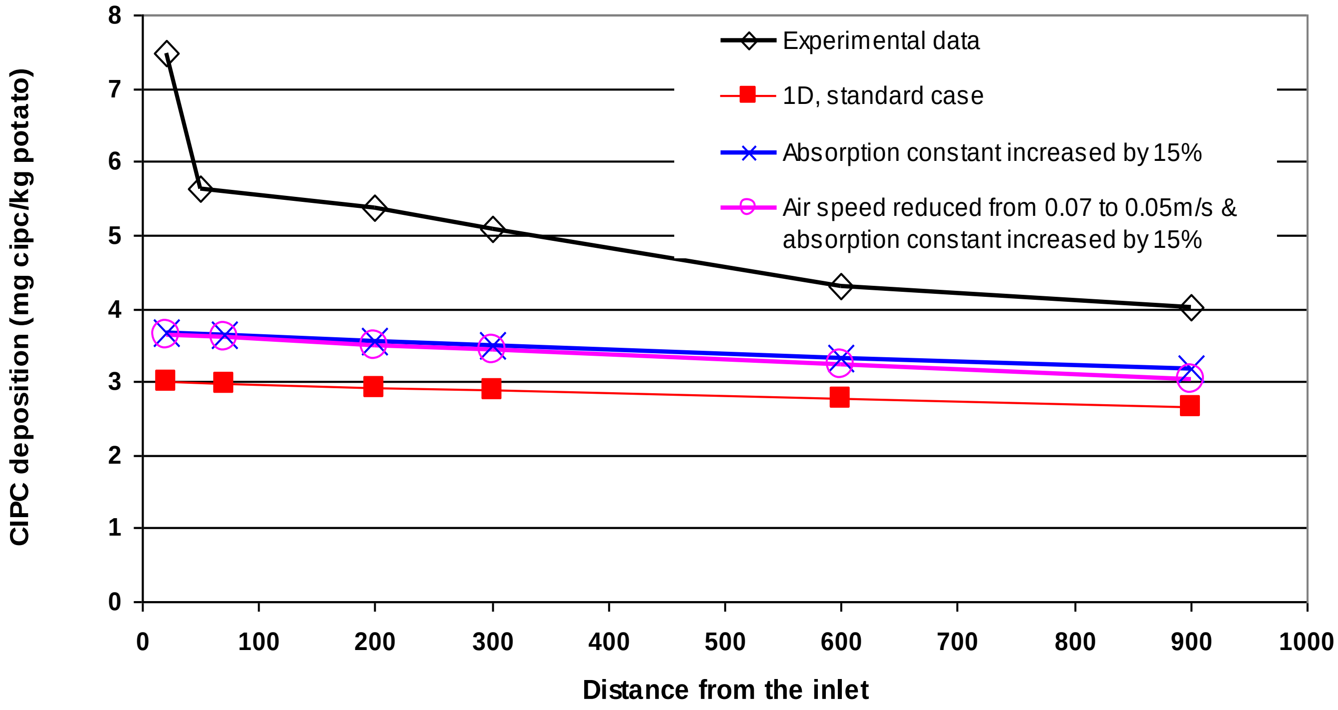


Figure 20. The influence of absorption coefficient and air velocity

on the predicted absorption

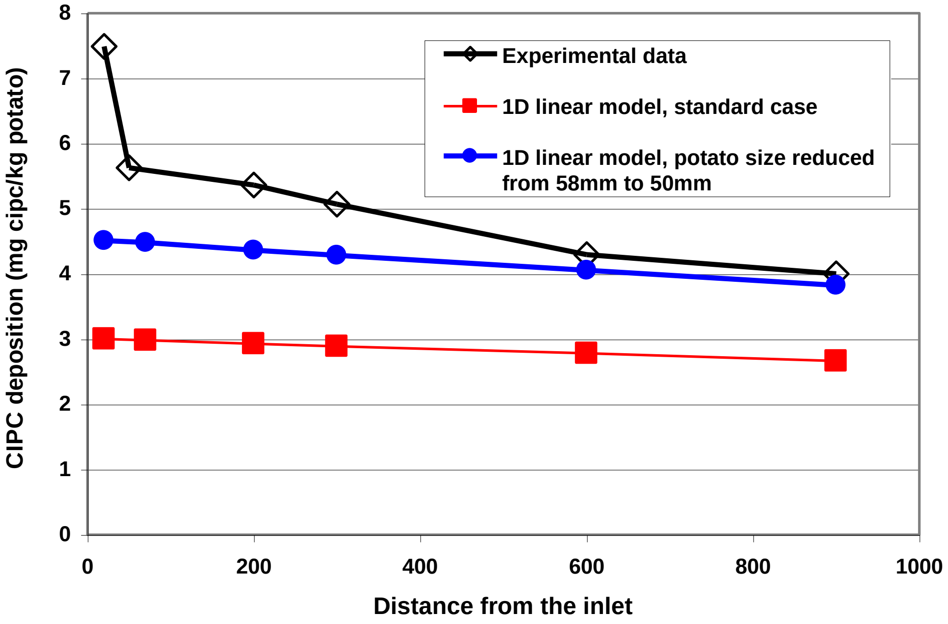


Figure 21. The influence of potato size on the predicted absorption (the low flow case)

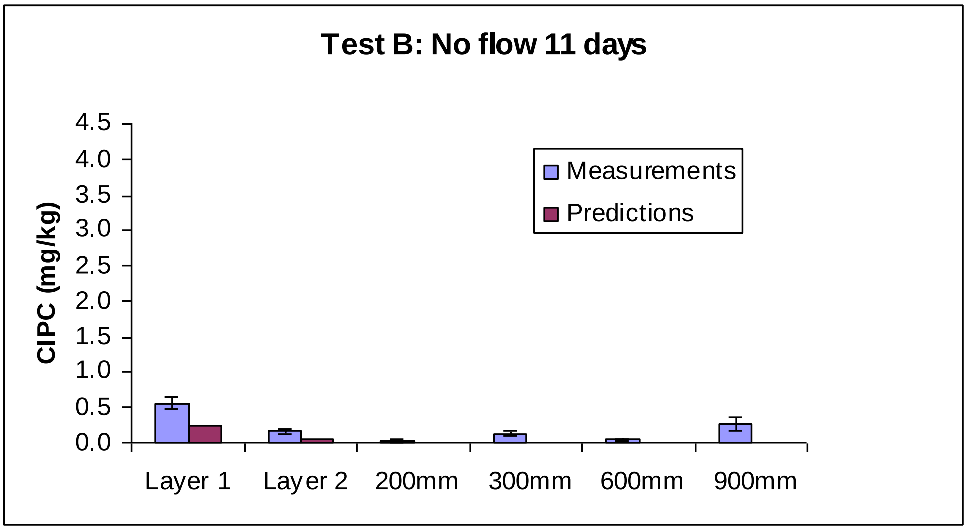
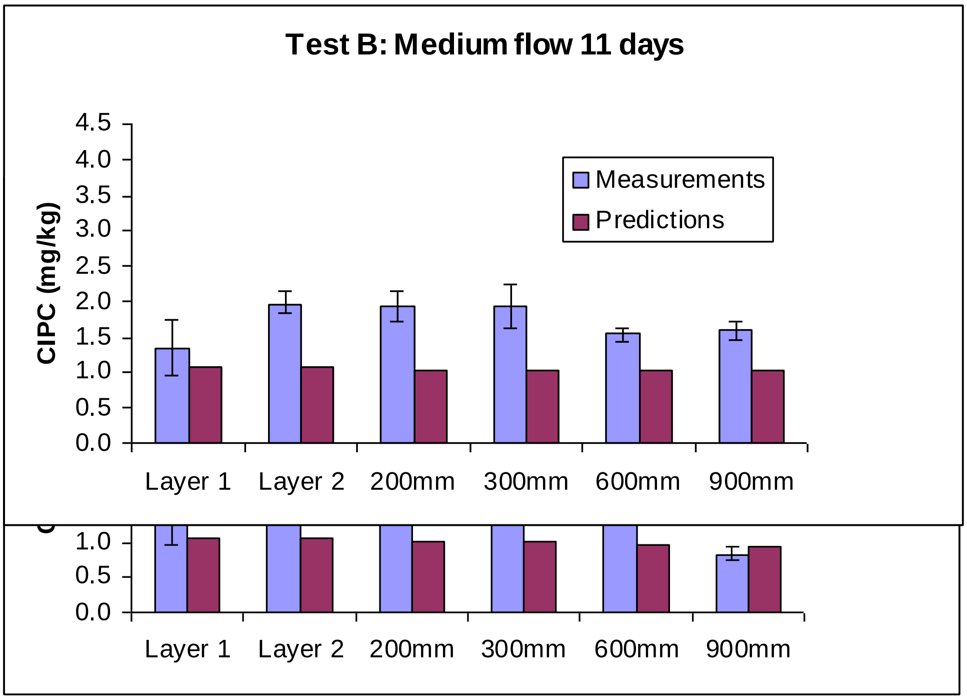


Figure 22(a). Comparing measured and predicted deposits

(Test B at 11 days)



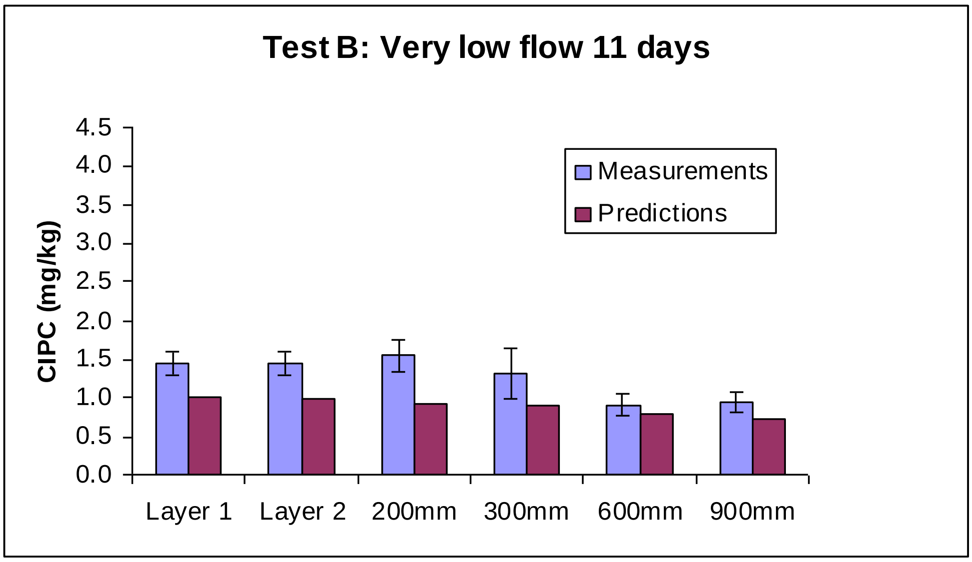


Figure 22(b). Comparing measured and predicted deposits (Test B at 11 days)

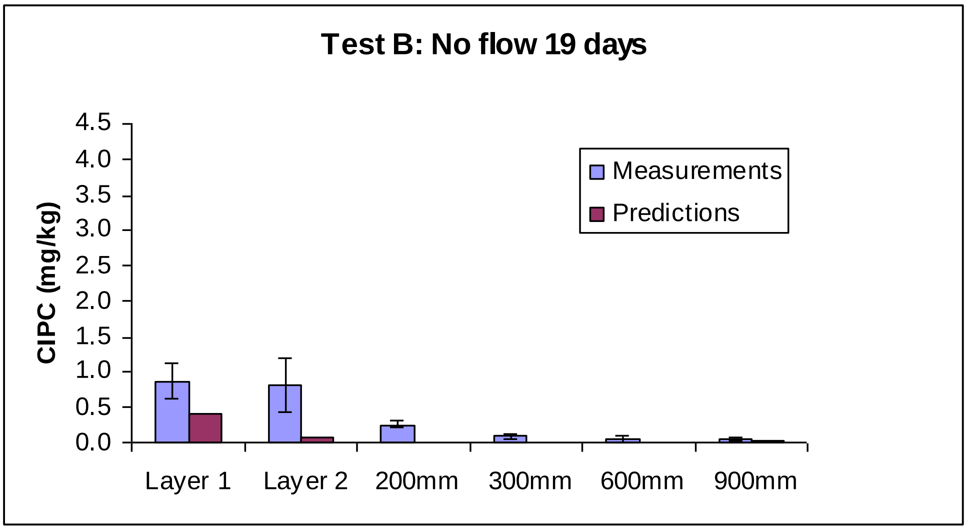
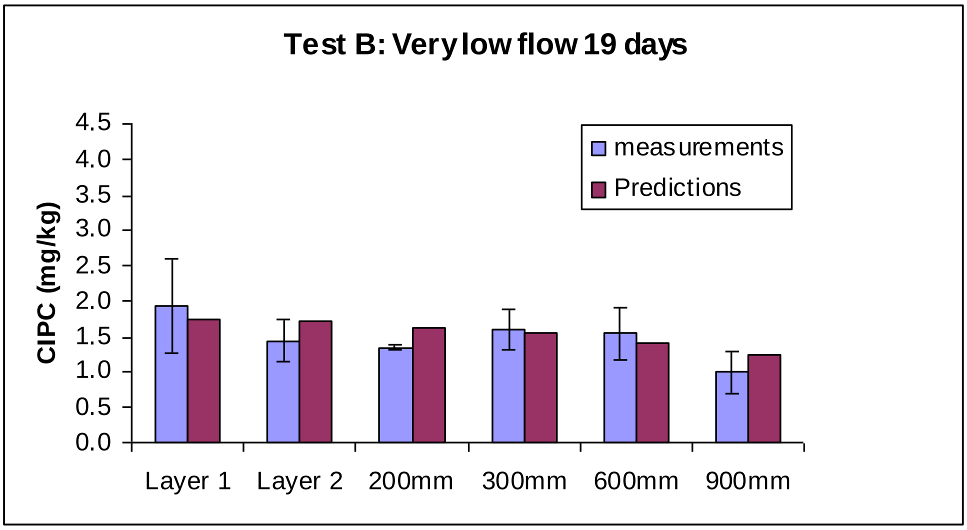


Figure 23(a). Comparing measured and predicted deposits
(Test B at 19 days)



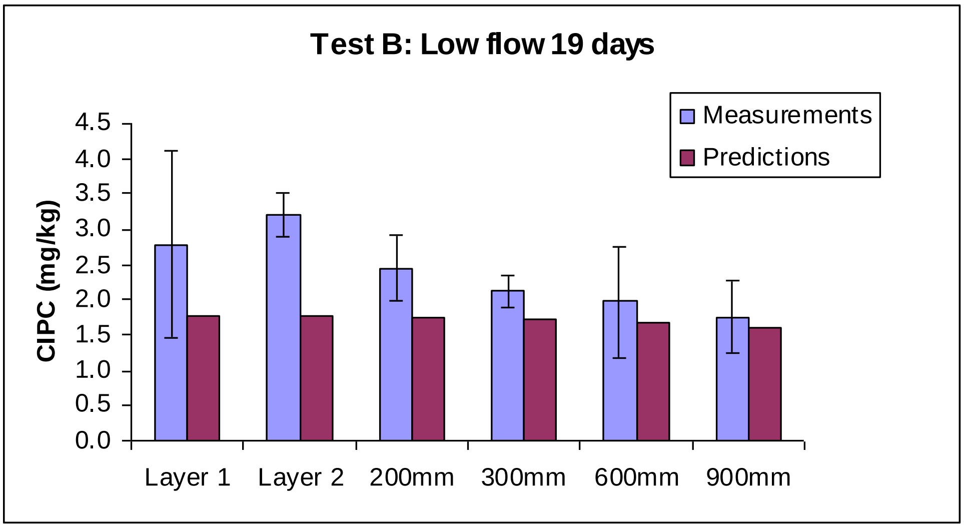
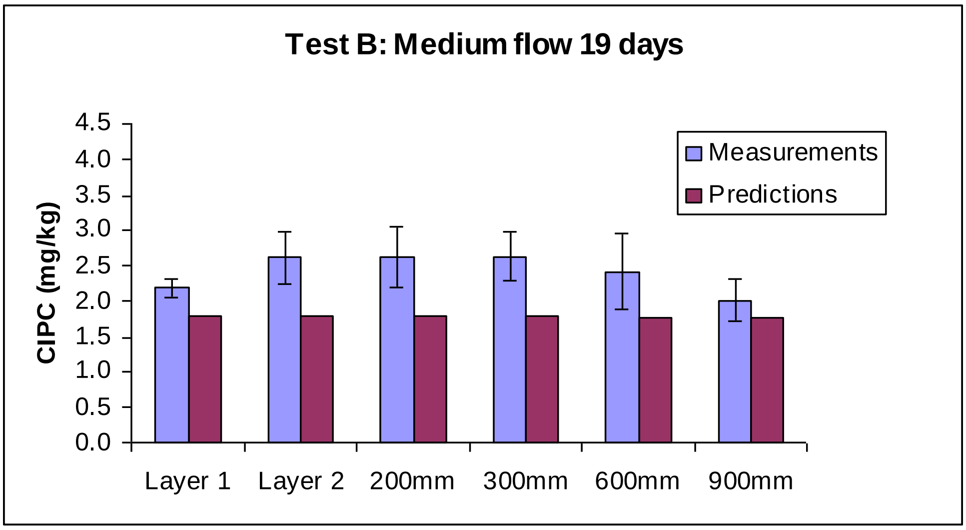


Figure 23(b). Comparing measured and predicted deposits (Test B at 19 days)



5.3 Conclusions

The differences between the predictions using the linear and exponential models are small. Because of the simplicity of the linear model, it was selected for the simulations of the experimental and commercial potato stores.

-The predicted and measured CIPC depositions are relative uniform crossing the packed potatoes when the velocity is higher than the case of ‘Very very low flow’, i.e. 0.02-0.03 m/s through the pipe. This is indicating a minimum air velocity required to achieve uniform vapour CIPC absorption through packed potatoes. In commercial stores, the height of potatoes inside a box is about 0.7 m, an air velocity of 0.03-0.05 m/s through the potatoes maybe is adequate to produce uniform absorption of vapour CIPC.

The accuracy of the predictions by the models developed depends on the accuracy of the parameters used and the assumptions made to develop the model. In general, the model has predicted the absorption satisfactorily against the results of the pipe test and should be further validated against measurements from potato stores.

6 Testing the model: 12-tonne potato stores

6.1 The model setup & input data

The ventilation system of the 12-tonne experimental store used for the study was such that air was circulated by a fan and was forced into the plenum through a throttle plate on top of it. The bypass duct was switched off during the tests to simply air movements. The ventilation rate was estimated to be 0.8 m^3/s by the SBEU team. Even though the store has a capacity of 12 tonnes, only 8 tonnes of potatoes were used in the tests and they were contained in eight boxes stacked in two vertical columns at the front of the plenum. An average potato diameter of 50 mm, a bulk density of 620 kg m^{-3} and a bulk porosity of 0.42 were used in the simulation.

The CIPC application port used for previous tests was sealed off in the tests for vapour CIPC. In the tests, the release of vapour CIPC at both store temperature (i.e. the cold source) and at high temperatures (i.e. the hot source) were investigated. However, due to lack of reliable data on the evaporation rate for the cold source, simulations were only done for the cases using the hot source. In these cases, CIPC was evaporated from a flask mounted in hot oil with controlled temperature. Hot vapour CIPC was released inside the plenum at a position where good mixing was generated by the airflow that was tested using smoke. The measured releasing rate of vapour CIPC was 0.154g/h, which was scheduled to release 70g CIPC into a store in 19 days. Even thought temperature is important for the release of CIPC using a hot source, especially in the region surrounding the releasing position, it is not thought be significant for the store and no heat transfer was included in the simulations presented below.

Figure 24 shows the computer model for the 12-tonne potato stores. The total number of cells representing the store was 73984 with 1920 cells used to represent each box (including the gap between the neighbouring boxes). The bottom of each potato box was formed by equally spaced wooden slats with only 15% of the total area available for the passage of air. Girding each box according to the gaps at the bottom would lead to a very large number of computational cells and consequently a very long computing time. In the model, the box bottoms were represented by coarse grids, the diffusivities of CIPC vapour were reduced in the bottom region of each box to only 15% of their free space values and additional momentum forces were used to represent the resistance of the slats to the air flow.

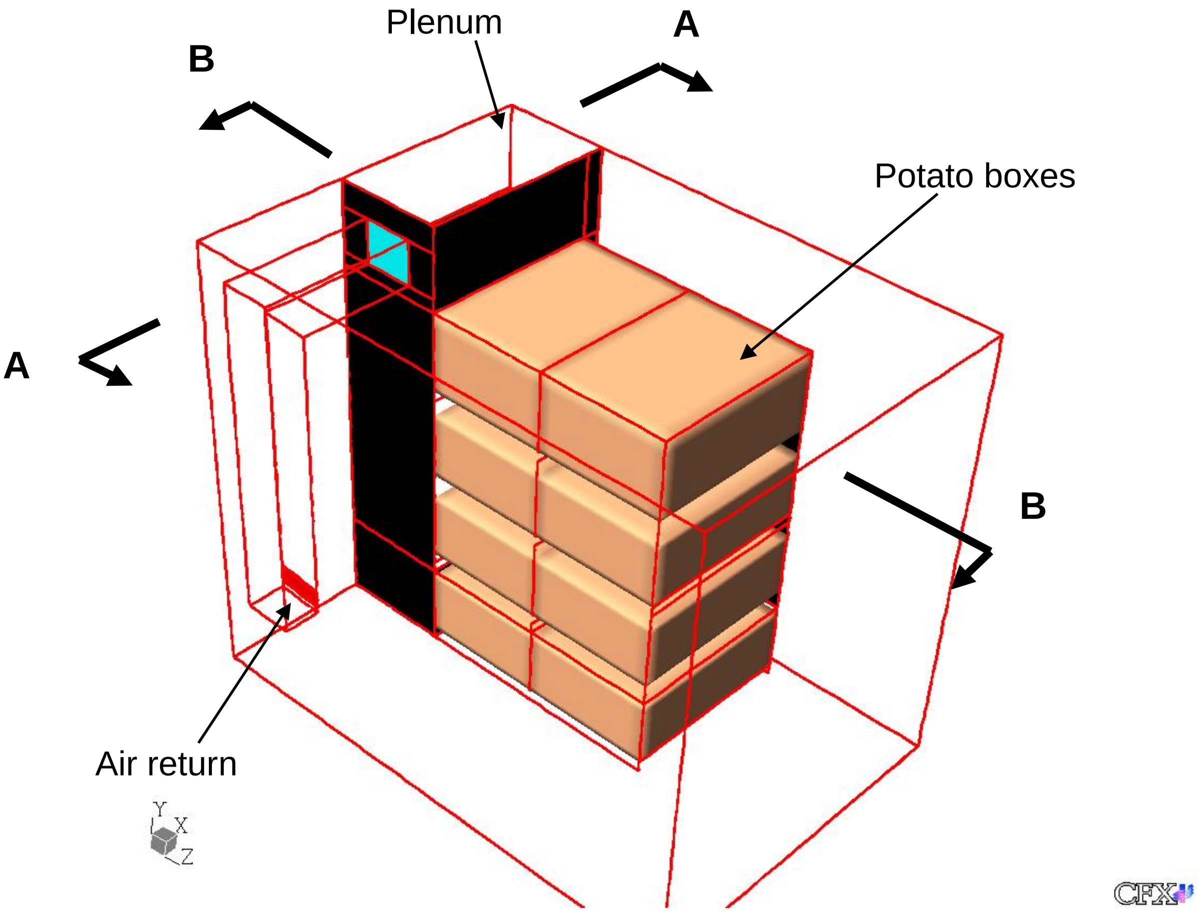


Figure 24. Computational model for the 12-tonne experimental store

The transfers of air and CIPC vapour in potato stores are transient processes so their governing equations need to be solved simultaneously at each time step and the time steps used have to be kept small to ensure solution accuracy and stability. In practice, it is not practical to simultaneously solve all the equations at every time step for the whole 19-day test period due to the huge computing time required. To balance the requirements of solution accuracy and speedy solutions, the simulation of each test case was done in three phases and extra simplifications were introduced in each phase to speed up the simulations.

- Phase 1: establishing flow patterns. The equations for air movements and CIPC transportation were solved simultaneously to the highest accuracy in this phase. The time step used at this phase was very small and the number of solution iterations for all equations at each step was large. This phase only represented the development of airflow in the store in the first 2-5 minutes from the start of the test in real time and CIPC was released at the start of this phase. To ensure the flow patterns were fully developed, the initial guess of the flow patterns in the store for the transient simulation were better as a steady state solution.

- Phase 2: establishing CIPC concentrations inside the store. In this phase, the flow patterns inside the store were assumed to be constant, and only the equation for CIPC transportation was updated at each time step to the highest accuracy. The time step and the number of solution iterations of the equation were kept the same as for phase 1. Because only one equation was solved, the simulation speed should have increased significantly. This phase normally represented the development of CIPC distributions in the store in the first 6-12 hours from the start of the test in real time.

- Phase 3: estimating CIPC depositions in the whole test period. In this phase, both the flow patterns and the distributions of vapour CIPC inside the store were assumed to be constant. CIPC depositions in long periods can be predicted in a reasonable time because of the simplifications.

The modelling strategies given above are suitable for both experimental and commercial stores with forced ventilation all the times. If the ventilation and the release of CIPC are operated on an on/off base, the three phases given above would have to be repeated for each of the on/off cycles to obtain accurate predictions.

All the equations were solved using the computational fluid dynamics package CFX4 (AEA Technology, Harwell, Oxford, UK) for the results given below.

6.2 The modelling results of the 12-tonne experimental stores

6.2.1 Airflow patterns and the distributions of vapour CIPC

At the start of the simulation (i.e. time equals zero), the store was assumed to have a uniform temperature of 10 ^{o}C and airflow patterns of a steady state simulation, no vapour CIPC was in the store at this time. In the simulation of Phase 1, the time step was 0.1 second and the duration of this phase was 2 minutes. Figures 25a & 25b show the predicted airflow on a vertical plane crossing the plenum (i.e. plane A-A as shown in Figure 24). The fast airflow through the throttle plate is generating a strong circulation inside the plenum as shown in Figure 25a. The colours in Figure 25b show the vapour CIPC concentrations and the place with the highest concentration is the CIPC releasing point. The strong circulation shown in Figure 25a is producing a good mixing of the released CIPC and this was observed while deciding this releasing point using smoke. The saturation concentration of vapour CIPC at 10 ^{o}C is around 0.1 μg/l and the predicted vapour concentration near to the releasing point is higher that the saturation value. This means that the circulation inside the plenum is not strong enough to disperse all the vapour CIPC released and CIPC particles or solid deposits maybe forming in the releasing regions in this test case.

Figures 26a & 26b show the predicted airflow pattern and the predicted deposition of vapour CIPC on a vertical plane along the centre of the potato boxes (i.e. plane B-B as shown in Figure 20) at the end of phase 1. At this early stage, the top box near to the plenum was having the highest CIPC deposition.

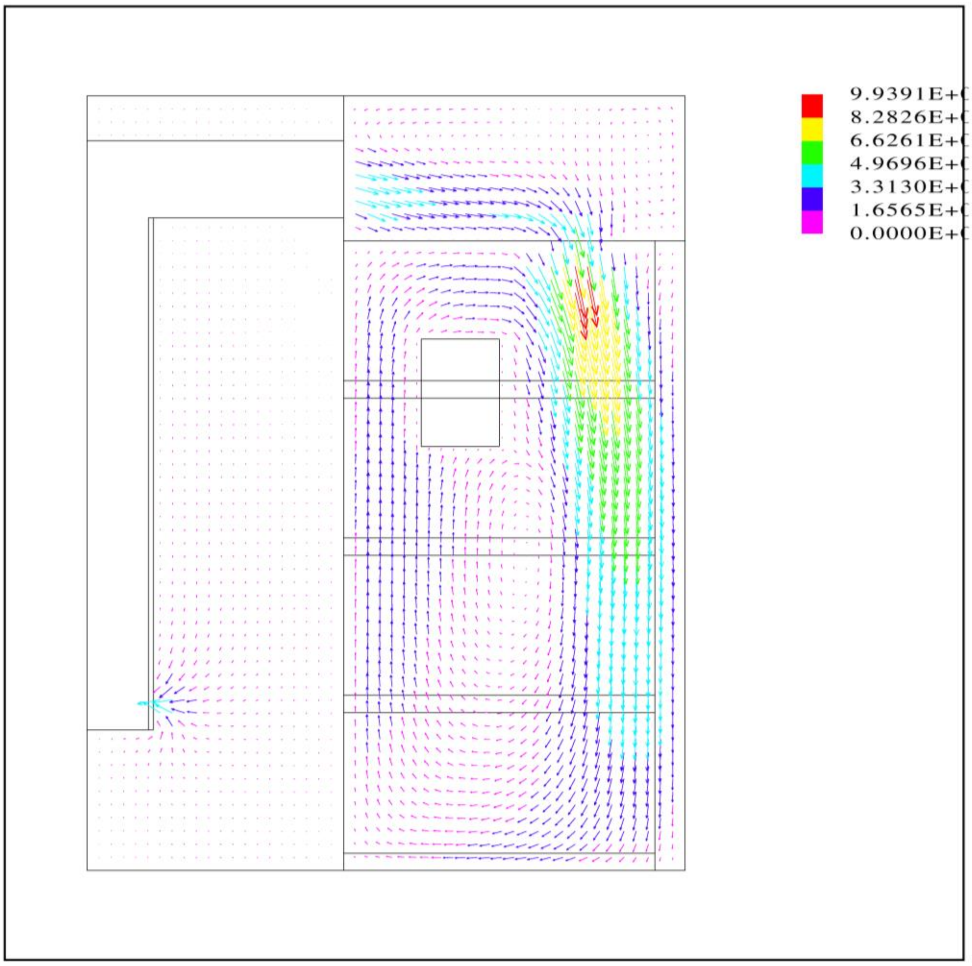
For all results presented so far, the equations of mass, momentum and CIPC movement were solved simultaneously at all time steps and 80 seconds of CPU time were required for each time step (0.1s) on a DEC Alphastation 250. A substantial computer power would be needed to simulate the 19-day test period and simplifications are needed.

6.2.2. CIPC depositions

Apart from being absorbed by potatoes, vapour CIPC is also being absorbed by walls & floor of the store, potato boxes and the ventilation system. These undesirable losses of vapour CIPC were treated in the same way as the potato absorption in the model, but have different absorption coefficients. Because no tests had been conducted in this study to quantify these undesirable absorptions and no published data were found about them, the absorption coefficients used in the models for these losses are "best guesses" and are only introduced to illustrate their influence on the treatment received by the potatoes.

Two simulations were carried out for each test case in this study, i.e. with and without CIPC absorption by the store walls and boxes. For the simulations including CIPC absorption by the walls and boxes, their absorption coefficients are assumed to be the same and equal to 15% of the value for potatoes. Figures 27 and 28 show the predicted CIPC depositions on plane B-B with and without absorptions by the wall and boxes during a 19-day period. In total, 70 grams of CIPC

Figure 25a Flow pattern on plane A-A (as shown in Figure 24, the colours of the arrows illustrate the magnitudes of air speeds and directions of the arrows show the direction of air movements)



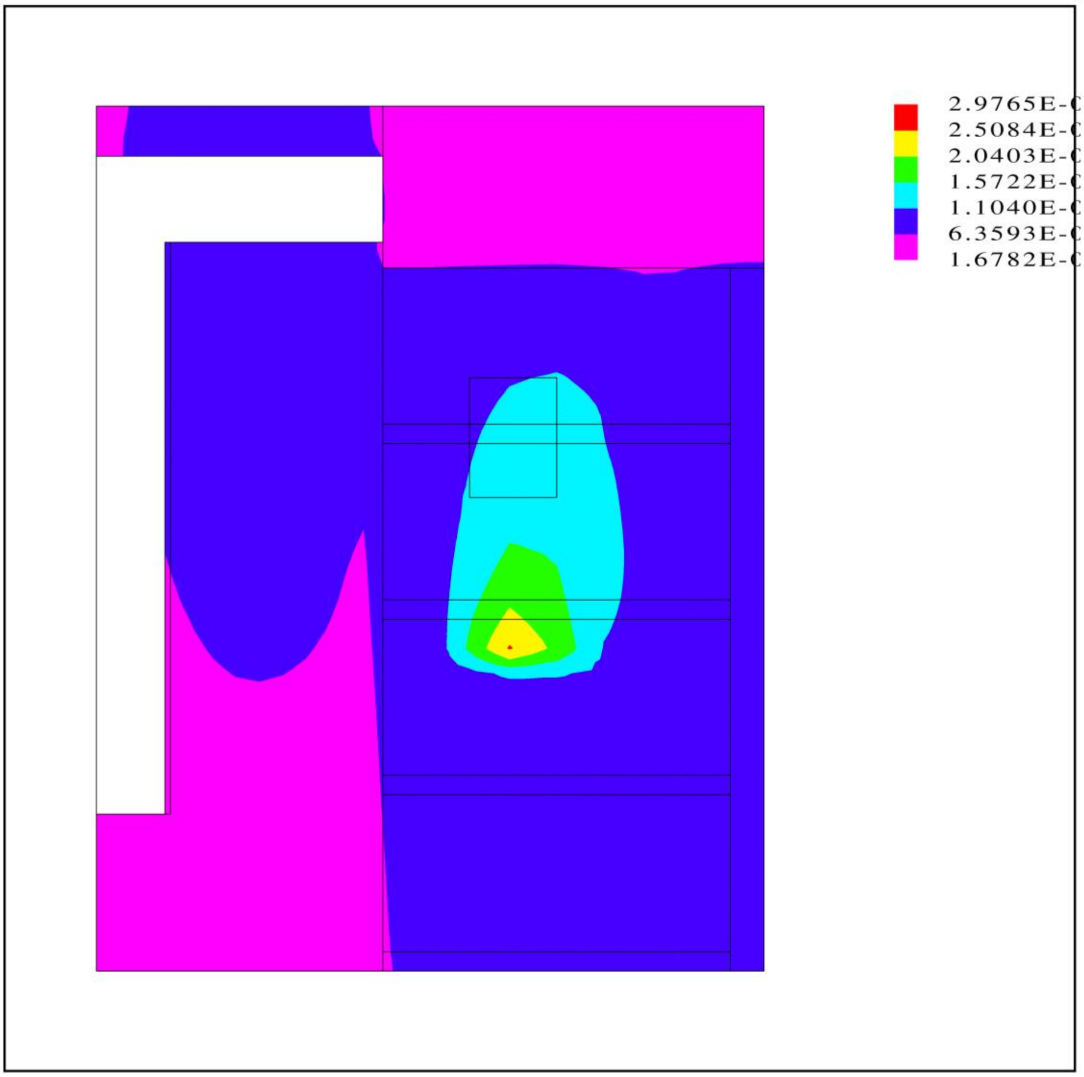
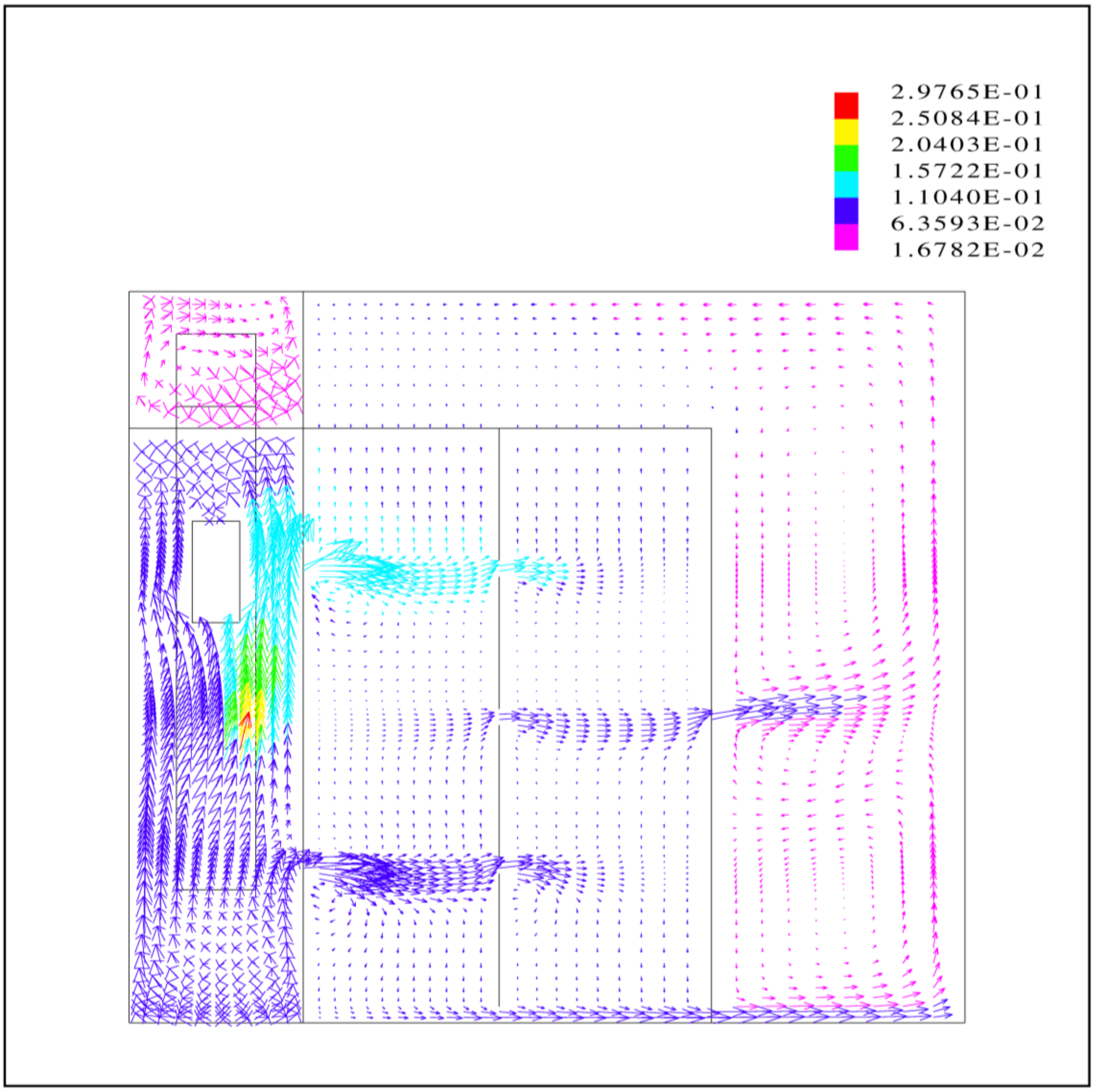


Figure 25b. Contours of vapour CIPC concentrations on plane A-A (as shown in Figure 24, vapour CIPC was released at the position with the highest vapour concentration)

Figure 26a Flow pattern on plane B-B (as shown in Figure 24) at the end of phase 1 of the simulation. The colours show concentrations of vapour CIPC and the arrows illustrate the directions of air movements.



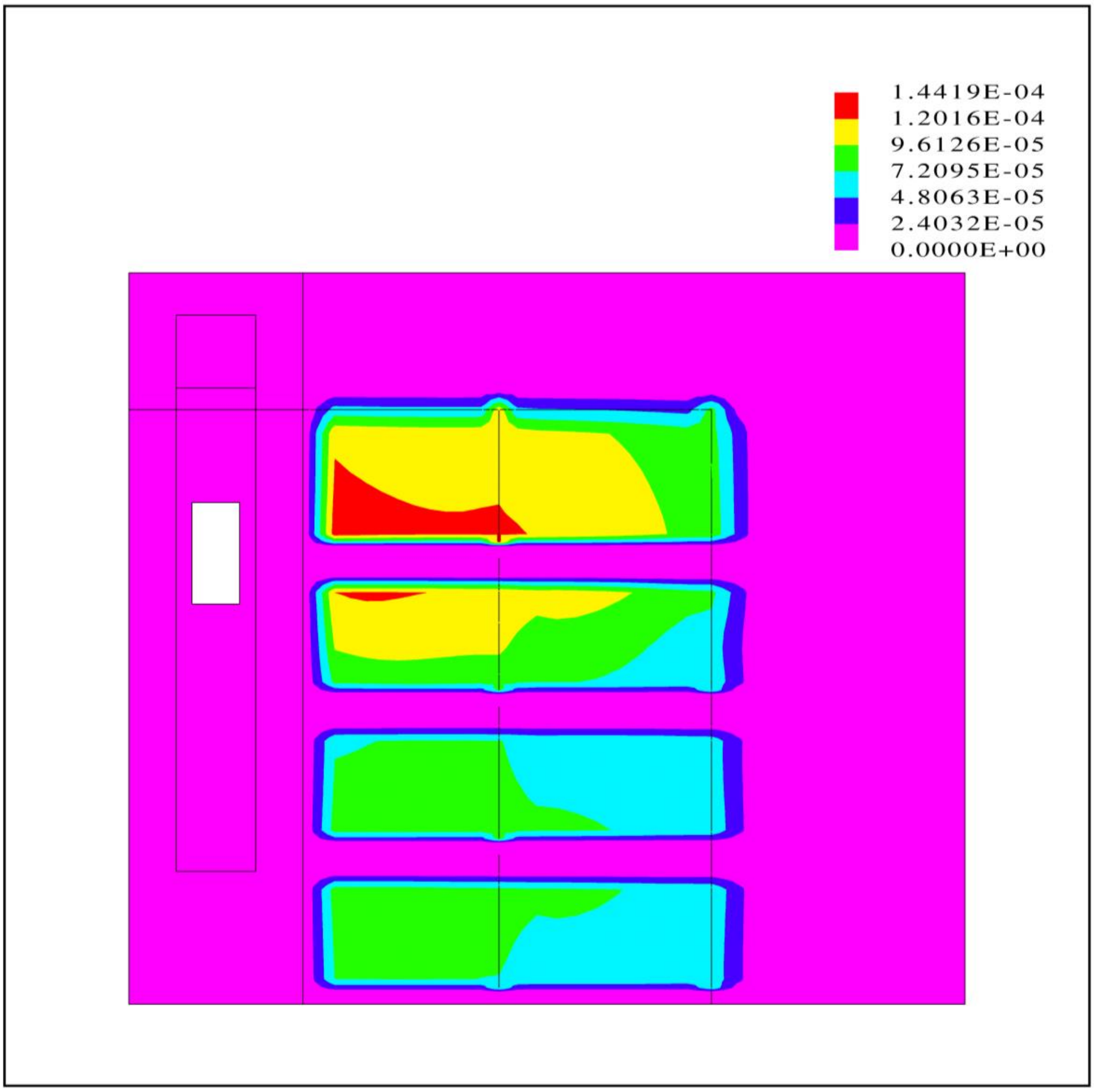


Figure 26b. Contours of vapour CIPC concentrations on plane B-B (as shown in Figure 24) at the end of phase 2 of the simulation

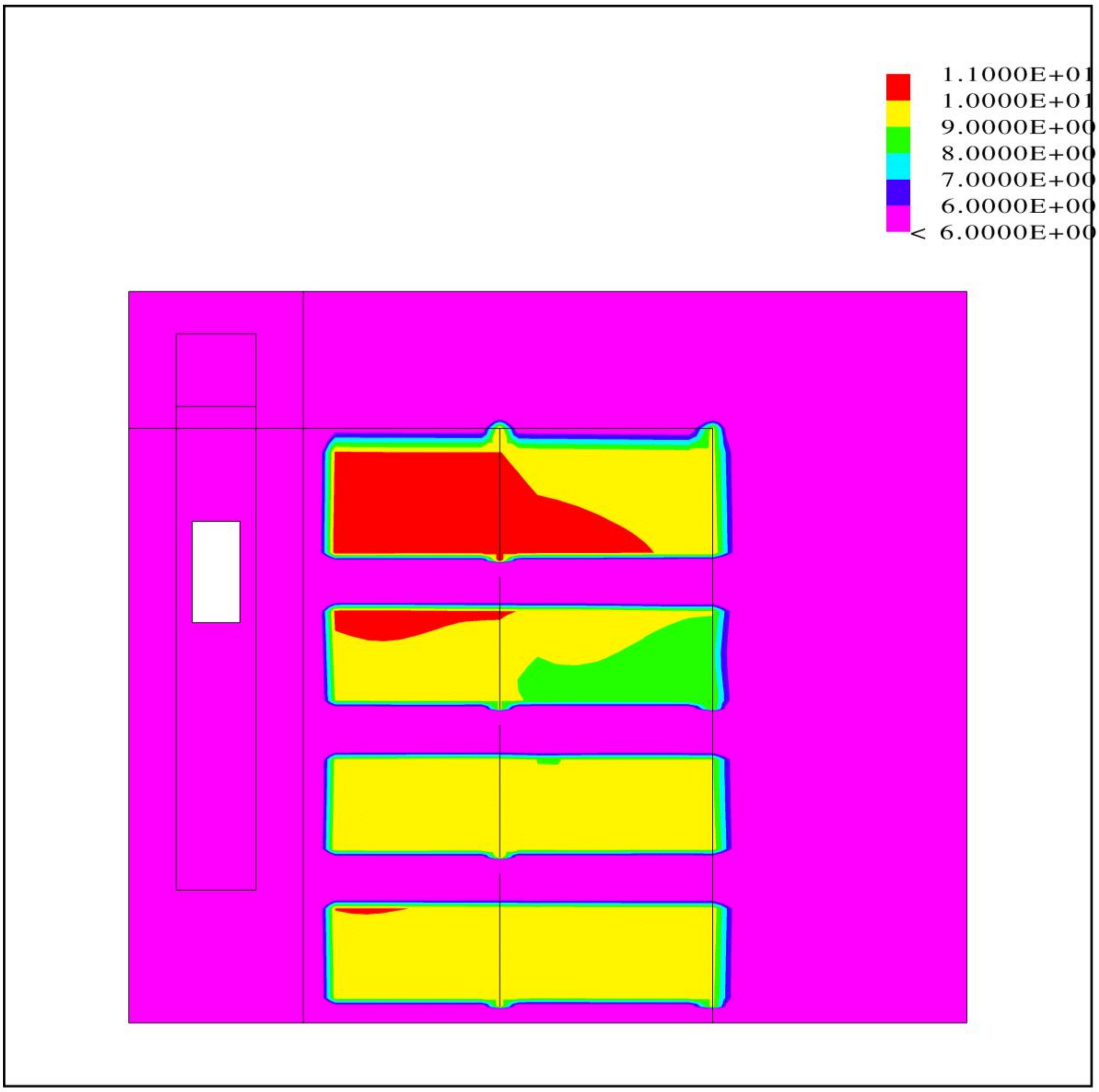


Figure 27. Contours of CIPC absorptions on plane B-B (as shown in Figure 24) in the 19-day period WITHOUT CIPC absorption by the store walls and potato boxes (Hot CIPC source, the releasing rate: 0.154g/h)

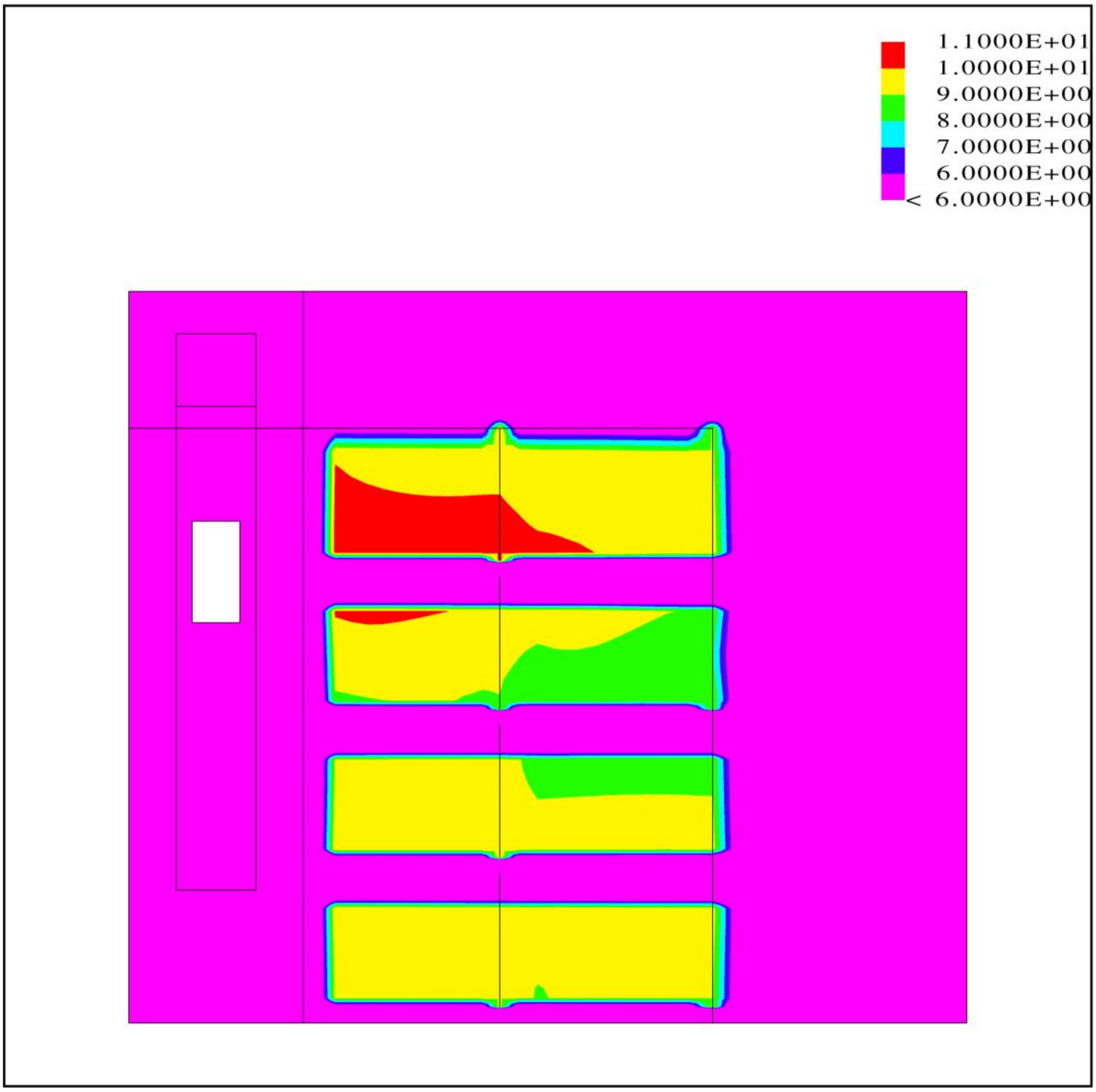


Figure 28. Contours of CIPC absorptions on plane B-B (as shown in Figure 24) in the 19-day period WITH CIPC absorption by the store walls and potato boxes (Hot CIPC source, the releasing rate: 0.154g/h)

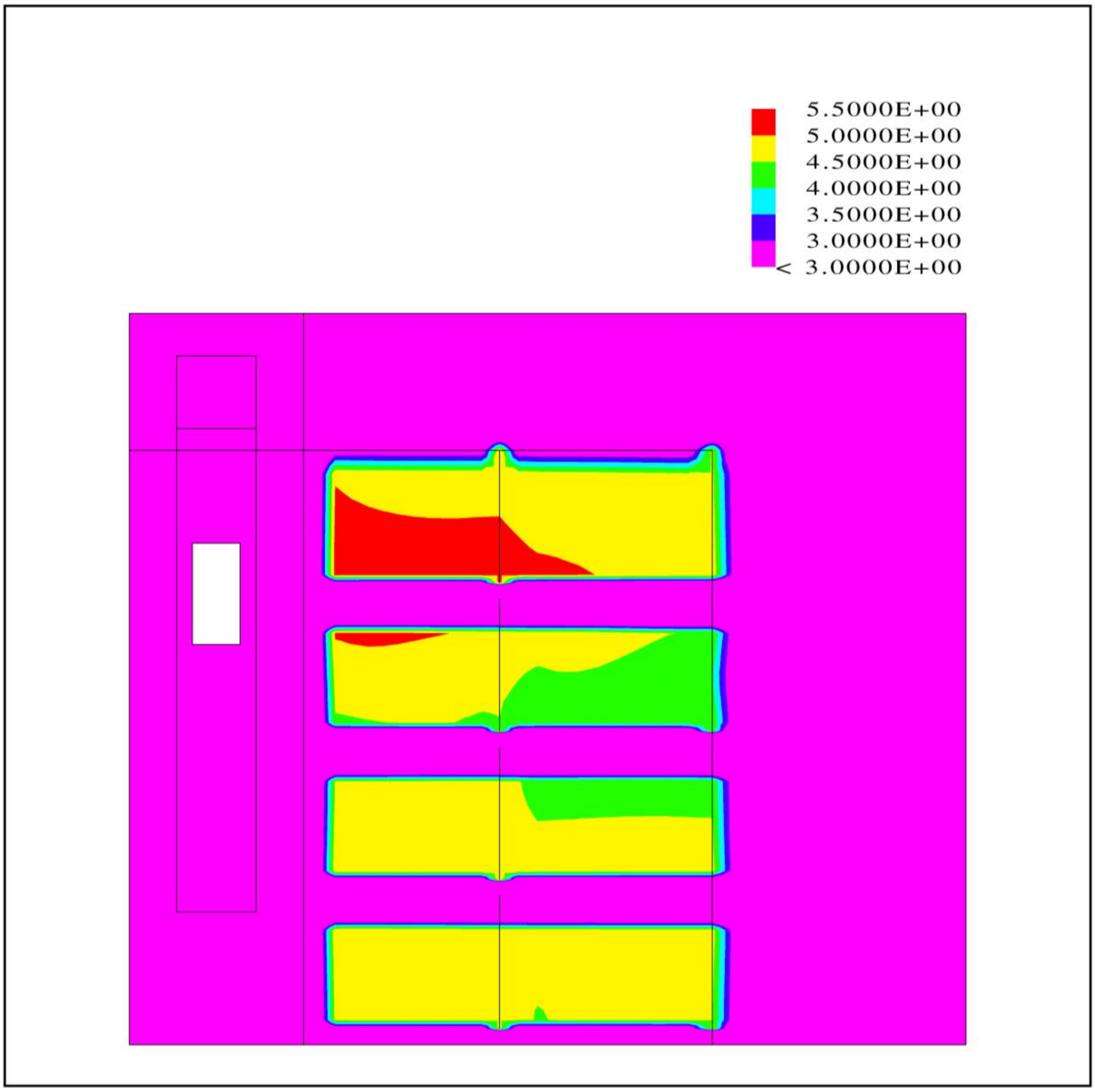


Figure 29. Contours of CIPC absorption on plane B-B (as shown in Figure 24) in the 19-day period with reduced CIPC releasing rate (Hot CIPC source, the releasing rate: 0.077g/h)

were released in to the store. Assuming all the CIPC was absorbed by potatoes, the averaged CIPC deposition on the potatoes would be 8.8 mg CIPC/kg potato. The predicted concentrations have not been directly related to the mass of potatoes in the store but do show that the range of deposit from largest to the smallest was +/- 16% of the mean value. It is therefore apparent that the treatments received by the potatoes using vapour CIPC is more uniform than that achieved using the conventional fogging approach.

Figure 28 shows the prediction including absorption by store walls and potato boxes. When their absorption coefficients were assumed to 15% of the coefficient of potatoes, the CIPC absorbed by store walls and potatoes boxes in 19 days is quite small and only accounts for 3.5% of the total CIPC released. The predicted highest and lowest CIPC absorptions in the store are therefore very similar to those with no absorption from the walls and boxes. Note that the absorption coefficient used for the walls and potato boxes were only estimated and could be significantly lower than the real values.

Figure 29 shows the predicted CIPC concentrations in the store for a substantially reduced release rate (0.077 g/h as against 0.154 g/h). This simulation was conducted because there was evidence from the practical experiment and model predictions that some of the vapour from the hot source was solidifying before it could be distributed in the store and therefore the effective release rate was well below the intended value. Comparing the results shown in Figures 28 and 29 indicates that the predicted distribution patterns within the store scale directly with release rate and there is little interaction between distribution patterns and source conditions.

6.3 Conclusions

- The computer models have been applied for a 12-tonne experimental store releasing vapour CIPC at high temperatures (i.e. the hot source).

- The predicted distributions of CIPC absorption for a 19-day are more uniform compared with the measured and predicted CIPC application using conventional hot fog in a similar store (i.e. Y. Xu and D. Burfoot, 2000).

- The predictions were made either without CIPC absorption by the store walls& floor and potato boxes or with an estimated absorption coefficient that could be significantly lower that the real value.

- The models still need to be adjusted based on measurements from the experimental store and from examples of full-scale commercial stores.

References

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Y. Xu, D. Burfoot & P. Huxtable, 2002, Improving quality of stored potatoes using computer modelling, Computers & Electronics in Agric., **34**, 159-171