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Multivariate analysis on simulated moisture damage emission to indoor air

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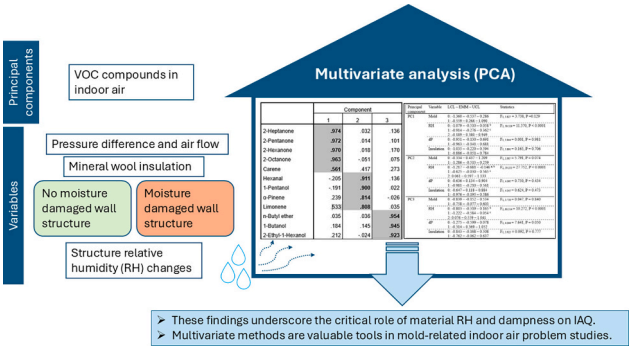
HIGHLIGHTS

- The RH was the most significant single factor influencing the VOC concentrations.
- 2-Pentanone, 2-hexanone, 2-heptanone, and 2-octanone were identified as MVOC.
- Pressure difference had minimal effect on IAQ because of opposite air flow effect.
- These findings underscore the critical role of material RH and dampness on IAQ.
- Multivariate methods are valuable tool in mold-related indoor air problem studies.

GRAPHICAL ABSTRACT



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ABSTRACT

Moisture damage in buildings is a significant source of indoor air problems, releasing e.g. volatile organic compounds (VOCs) and microbially produced VOCs (MVOCs), which can cause unpleasant odors and health symptoms. However, interpreting MVOCs as indicators of mold is challenging due to their various sources and limitations in analytical methods.

The objective of this study was to identify the most critical factors influencing VOC emissions from moisture-damaged wall structures into the indoor environment via structural air leakages. The research was conducted using the VTT Indoor Air Quality (IAQ) Simulator and analyzed with Principal Component Analysis (PCA). The IAQ simulator was used to investigate the transport of airborne impurities from mold-contaminated wall structures in realistic building conditions and the systematic manipulation of key environmental parameters. The resulting dataset was subjected to multivariate analysis to identify the most influential factors contributing to IAQ degradation in moisture-damaged structures.

The key conclusions revealed that material relative humidity was the most significant single factor affecting all VOC concentrations; higher humidity consistently increased emissions. Four specific ketones (2-pentanone, 2-hexanone, 2-heptanone, and 2-octanone) were clearly identified as originating from microbial growth, with their concentrations being significantly higher in the presence of active mold growth. Pressure differentials had only a borderline effect on gypsum board emissions, while the insulation layer showed no significant impact on any of the identified VOC components. These findings underscore the critical role of relative humidity in

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determining indoor VOC profiles and highlight the value of multivariate methods in assessing mold-related indoor air problems.

1. Introduction

Indoor air quality (IAQ) in non-industrial buildings is a critical determinant of human well-being and health, with suboptimal IAQ potentially leading to a range of symptoms and adverse health outcomes. Moisture damage is one of the biggest causes of indoor air quality problems, and as the climate changes, the moisture load on buildings will also increase, creating new risks for moisture damage. Energy efficiency repairs required by buildings can also cause moisture damage if done incorrectly. As individuals spend a substantial majority of their time indoors, exceeding 90% (Kleipeis et al., 2001) - the quality of the indoor environment has become increasingly significant for public health (Choi et al., 2024). IAQ is shaped by a complex interplay of environmental, structural, and human behavioral factors that collectively influence occupant health and comfort.

A significant challenge to IAQ arises from moisture damage and microbial contamination in building structures, which are recognized as major contributors to indoor air problems (Husman, 1996; WHO, 2009). Such contamination often leads to the emission of microbial volatile organic compounds (MVOCs) (e.g. Claeson, 2006, Fiedler et al., 2001, Korpi et al., 1998, Schleibinger et al., 2005, Schleibinger et al., 2008, Wilkins et al., 2000). MVOCs are compounds produced during the metabolism of fungi and bacteria from nutrient substrates (Korpi et al., 2009). In case of moisture damage, both building materials and fungal activity emit VOCs, and cause health effect e.g., unpleasant odor, irritation in eyes and respiratory track (Korpi et al., 2009; Saijo et al., 2004).

MVOCs encompass a wide range of organic molecule classes, including ketones, aldehydes, alcohols, and hydrocarbons (Korpi et al., 2009; Korpi et al., 2006). More than 200 individual MVOC compounds have been identified in laboratory studies (Korpi et al., 2009). However, it is important to note that no single MVOC compound is exclusively microbial in origin or specific to certain microbial species, as they can also have other sources in the environment, such as building materials, human activity, traffic, food, and smoking (Thrasher and Crawley, 2009). Korpi et al. (2009) reviewed MVOC related studies in updated version of a criteria document from the Nordic Expert Group for Criteria Documentation of Health Risks from Chemicals, which was initially published in 2006. Based on this review, most often reported microbial metabolites in living environments were alcohols (2-methyl-1-propanol, 3-methyl-1-butanol, 3-methyl -2-butanol, 2-pentanol, 3-octanol, 1-octen-3-ol, 2-octen-3-ol), furan derivatives (3-Methylfuran), ketones (2-hexanone, 2-heptanone, 3-octanon), terpenoids/Terpenes (2-methyl-isoborneol, geosmin), pyrazines (2-isopropyl-3-methoxypyrazin), and sulfur compounds (dimethyl disulfide).

These compounds are volatile metabolites from microorganisms (MVOC), and they are supposed to indicate the hidden mold growth in buildings. This assumption proved to be challenging because of low concentrations and variety between fungal and bacterial species, relative humidity, and growth media (Korpi et al., 1998; Sunesson et al., 1995), but also other sources of the same compound.

Particularly in cold-climate countries, such as Nordic countries, modern energy-efficient construction practices and increasingly airtight building envelopes, while designed to enhance thermal comfort and reduce energy consumption, can inadvertently lead to the accumulation of indoor pollutants if not adequately ventilated (Hägerhed-Engman et al., 2009). Buildings are typically designed to maintain a slight negative indoor pressure (−2 to −5 Pa) to prevent warm, moist indoor air from migrating into the building envelope, where it could condense and cause moisture damage. However, this negative pressure can also draw in air from unintended sources—such as wall cavities, crawl spaces, or the ground—especially when the building envelope is not properly sealed or ventilation system is imbalanced (Hachem et al., 2009, Airaksinen et al., 2004). These pressure differences can drive air—and with it, airborne pollutants such as MVOCs, fungal spores, and fibers—through cracks, joints, and utility penetrations.

In buildings with mechanical exhaust ventilation, the absence of controlled intake air inlets can lead to uncontrolled air infiltration through structural leakages. Similarly, imbalances in mechanical supply and exhaust ventilation systems may cause pressure differences that drive unintentional airflow through the building envelope (Saini et al., 2021; Zhang et al., 2020). Variations in ventilation operation between day and night can further exacerbate these pressure differences, potentially leading to air movement between building zones or from the exterior into the interior, thereby transporting pollutants indoors (WHO, 2021). In Finnish residential buildings, wintertime temperature differences between indoor and outdoor air can exceed 40 °C, leading to pressure differentials as high as −20 Pa (Leivo et al., 2015). Pressure differentials are influenced also by stack effect, where warm air rises and creates negative pressure on lower floors and positive pressure on upper floors, and wind pressure, which varies across building facades depending on wind direction and speed. The stack effect is particularly

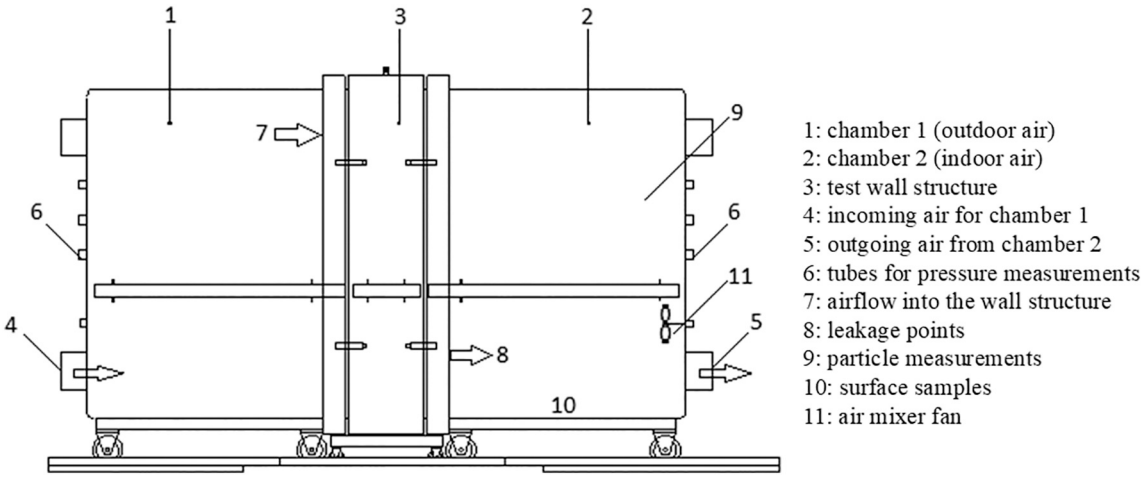

Fig. 1. The principle of the IAQ simulator.

Fig. 2. Test wall structure opened. At the beginning of the test, five wooden laths were placed vertically in a steel basin inside the wall structure to which water was added at the beginning of the test. There was visible mold growth on the surface of the wood in the picture. The variation in the relative humidity and temperature of the wood material was measured with a surface sensor taped to the surface of the wood.

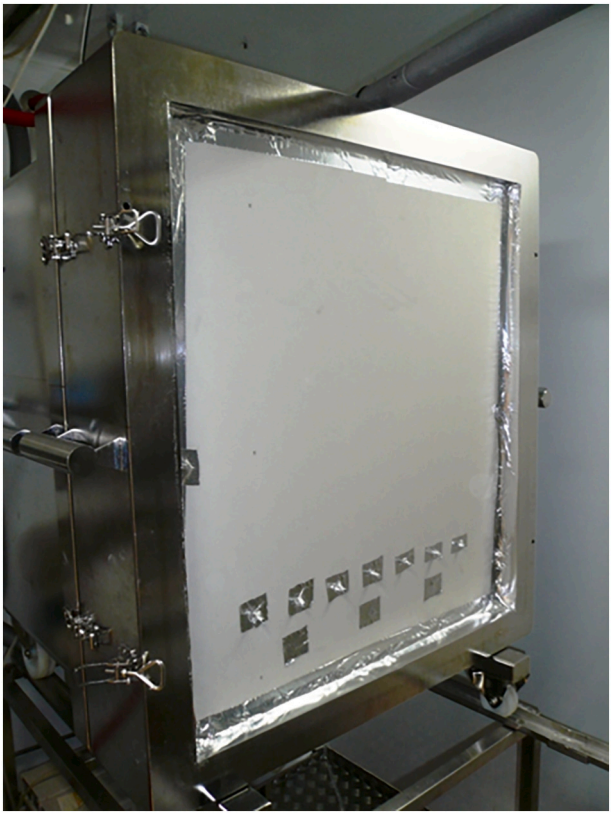

Fig. 3. Test wall closed with gypsum board from the indoor air chamber side. Air leakage holes are visible in the gypsum board.

relevant in multi-story buildings, where it can cause vertical air movement that redistributes pollutants between floors.

In this study, a novel approach to indoor air quality (IAQ) assessment was developed by combining the VTT Indoor Air Quality Simulator with multivariate statistical methods. As part of the Microdiverbuild project (2012–2014), the IAQ simulator was used to investigate the transportation of airborne impurities from mold-contaminated wall structures under controlled variations in material relative humidity and pressure differentials across the building envelope. The experimental setup enabled the simulation of realistic building conditions and the systematic manipulation of key environmental parameters. The resulting dataset was subjected to multivariate analysis to identify the most influential factors contributing to IAQ degradation in moisture-damaged structures.

2. Materials and methods

2.1. Experimental setup

The Indoor Air Quality (IAQ) simulator, developed at VTT Technical Research Centre of Finland (Paavilainen, 2005; Paavilainen et al., 2007), was used to investigate emissions from multilayer wall structures. This system provides a method for assessing air leakage and indoor environmental quality, and it is based on ISO 16000-9 (ISO, 2006). The principle of the IAQ simulator is presented in Fig. 1.

The simulated wall structure consisted of square-shaped (0.72 m^2) wood-framed assembly covered with gypsum board. Air leakage routes were created by drilling 6 mm holes into the gypsum board, and five vertical pine sapwood laths were placed between the boards (Fig. 2). Wood laths were placed in a steel basin inside the wall structure to which one liter of tap water was added at the beginning of the test. The test wall was modified between measurement setups: the drilled holes were either opened or sealed to vary the pressure difference and corresponding air leakage rate. All other potential leakage paths, particularly at the board edges, were carefully sealed with low-emitting aluminum tape (Fig. 3). Test runs were conducted both with and without mineral wool insulation.

The calculated air leakage rate of the wall structure was 1.4 m^3/h under low pressure differences (−2 to −4 Pa) and 0.6 m^3/h under higher pressure differences (−16 to −21 Pa). The air exchange rate in the IAQ simulator was maintained at 1.0 h^{-1}, with an incoming airflow of 8 L/min. Summary of the experimental conditions is presented in Table 1. The incoming air was filtered for particles and volatile organic compounds (VOCs) (<20 μg/m^3) and humidified to ensure clean and stable air conditions. All internal surfaces of the chamber and test structures were cleaned with steam and 70% ethanol before and after each test. Chamber blank samples were collected to confirm sufficiently low background VOC concentrations.

Mold exposure was simulated by inoculating both sides of the pine laths with a fungal suspension, followed by incubation under high humidity conditions for 4–6 weeks. The inoculated species included *Aspergillus versicolor* (D-96660), *Penicillium brevicompactum* (ATCC 58606), *Chaetomium globosum* (D-81079), *Cladosporium sphaerospermum* (D-88330), *Paecilomyces variotii* (D-83214), and *Trichoderma viride* (D-091397). The microbial suspension consisted of a mixture of six common mold species typically found in moisture-damaged building materials, simulating a representative microbial exposure. Pine laths without microbial inoculation were used as controls. Material samples from wood were taken before and after every test and analyzed with both cultivation and quantitative PCR (Polymerase Chain Reaction).

Table 1
Summary of the experimental conditions, including inoculated mold on sapwood material, relative humidity (RH) of the sapwood, pressure differences between the indoor and outdoor chamber, and the calculated leakage rates.

Case	Inoculated mold on sapwood (yes/no)	Follow-up time (days)	Wood material RH (%)	Pressure difference (average), Pa	Leakage rate (m^3/h)[a]	Leakage rate (m^3/h m^2)[a]
Minor pressure difference without mineral wool insulation	No	13	100 → 41	−2	1.4	2.0
	Yes	13	100 → 45	−4	1.4	2.0
Major pressure difference without mineral wool insulation	No	7	45 → 40	−16	0.6	0.9
	Yes	7	93 → 46	−21	0.6	0.9
Minor pressure difference with mineral wool insulation	No	13	100 → 50	−3	1.4	2.0
	Yes	13	100 → 48	−2	1.4	2.0
Major pressure difference with mineral wool insulation	No	13	97 → 52	−19	0.6	0.9
	Yes	13	100 → 50	−19	0.6	0.9

[a] Computational.

2.2. Sampling and analyses

Volatile organic compound (VOC) samples were collected from the chamber air using two parallel Tenax TA® adsorbent tubes, in accordance with ISO 16000-6 (ISO, 2004). The size of VOC samples varied between 2 and 6 L. The tubes were analyzed by thermal desorption–gas chromatography/mass spectrometry (ATD-GC/MSD, Agilent Technologies, Santa Clara, CA, USA) in SCAN mode, and the results were quantified as toluene equivalents. Compounds between hexane and hexadecane were analyzed. The results from the parallel samples were treated as individual data points in the statistical analyses.

The VOC compounds detected (above the detection limit) in these simulations were selected as the target VOCs. The following target VOCs were included in the statistical analysis: 1-butanol, 2-pentanone, 1-pentanol, 2-hexanone, hexanal, *n*-butyl ether, 2-heptanone, α-pinene, 2-octanone, carene, 2-ethyl-1-hexanol, and limonene. The detection limit for individual compounds was 2 μg/m^3.

The relative humidity (RH) and temperature of the wood material and chamber air (both indoor and outdoor) was measured using a sensor with a datalogger (Tinytag TV-4506, Gemini Data Loggers Ltd., UK). Wood surface sensor was located 10 cm from the bottom of the lath, while air sensors were placed near the chamber floor. Pressure differences between the chambers were continuously monitored using a SwemaFlow 300 (SWA10, Swema AB, Sweden).

2.3. Statistical analyses

Principal component analysis (PCA) creates composite variables by combining correlated original variables into fewer, new, uncorrelated variables (principal components) that capture most of the data's variance, reducing dimensionality while retaining key information. In this study, principal component analysis with varimax rotation and Kaiser normalization was used to identify key factors influencing indoor air quality in the presence of air leakage from mold-contaminated wall structures. The analysis evaluated the influence and correlations of relative humidity, pressure difference, mineral wool insulation, and

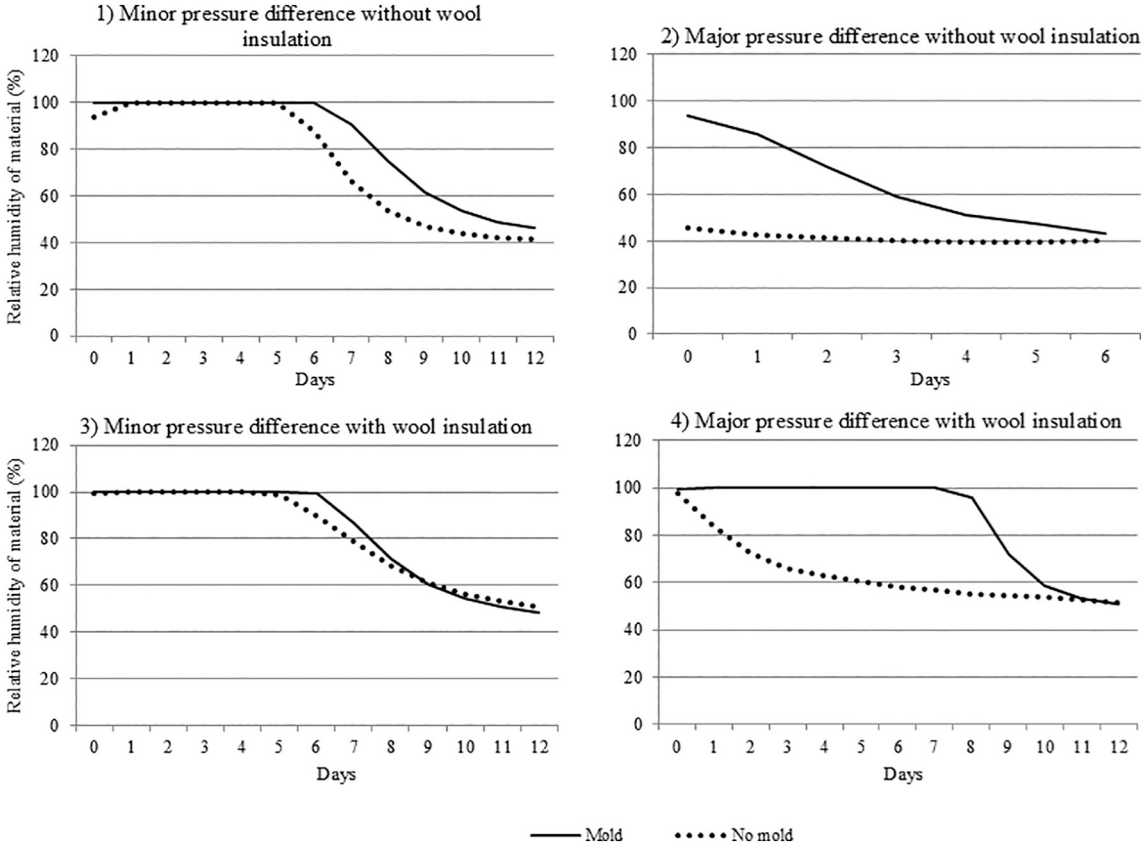

Fig. 4. Relative humidity (RH) of wood material changes during test runs.

Table 2
VOC compounds from test run with minor pressure difference without mineral wool insulation. The column colors (dark grey, light grey, white) indicate the moisture level (relative humidity, RH%) on the sampling day.

	Day 1 (μg/m^3)		Day 3 (μg/m^3)		Day 6 (μg/m^3)		Day 10 (μg/m^3)		Day 13 (μg/m^3)	
Compound	No mold	Yes mold	No mold	Yes mold	No mold	Yes mold	No mold	Yes mold	No mold	Yes mold
1-Butanol	2	3	3	2	<2	2	<2	5	<2	<2
2-Pentanone	<2	197	<2	138	<2	125	<2	11	<2	7
1-Pentanol	8	9	60	7	32	6	4	<2	3	<2
2-Hexanone	<2	35	<2	22	<2	24	<2	2	<2	<2
Hexanal	27	11	44	4	34	3	3	2	3	2
n-Butyl ether	<2	3	<2	2	<2	<2	<2	6	<2	<2
2-Heptanone	<2	78	5	53	3	60	<2	6	<2	3
α-Pinene	66	65	103	27	393	140	25	14	23	12
2-Octanone	<2	47	<2	38	<2	43	0	10	<2	6
3-Carene	14	26	17	11	63	26	5	6	5	5
2-Ethyl-1-Hexanol	5	8	6	5	4	5	<2	9	2	3
Limonene	<2	<2	13	4*	19	6*	2	<2	<2	2*
Material RH (measured)	90-100 %				60-90 %	90-100 %	40-60 %			

[a]Only in one of two samples.

VOC concentrations on mold detection.

The same 13 VOCs listed above were used to construct the principal components. Using mixed models with setup as a random factor, components with eigenvalues greater than 1 were compared with categorical variables: mold presence (yes/no), material relative humidity (RH: 40–60%, 60–90%, 90–100%), pressure difference (minor/major), and insulation presence (yes/no). The RH categories represent:

- Dry material (RH 40–60%), where mold growth is not possible,
- Moist material (RH 60–90%), where moisture may limit mold growth, and
- High moisture material (RH 90–100%), where moisture does not limit mold growth.

PCA and mixed model analyses were conducted using IBM SPSS Statistics 21. Results are presented with 95% confidence intervals.

3. Results

3.1. Relative humidity and temperature

The relative humidity (RH) of wood material changed from wet to dry during the test runs. At the beginning of the test run, water was added to the bottom parts of laths and water was absorbed into wood. The humidity changed during dehydration of water first from the tube and slowly from wood material. RH was 100% at the beginning in most of the test runs. In few cases, RH 100% was not achieved, or wood material dried out very quickly. This may be caused by differences in

Table 3
VOC compounds from test run with major pressure difference without mineral wool insulation. The column colors (dark grey, light grey, white) indicate the moisture level (relative humidity, RH%) on the sampling day.

	Day 1 (μg/m3)		Day 3 (μg/m3)		Day 6 (μg/m3)	
Compound	No mold	Yes mold	No mold	Yes mold	No mold	Yes mold (Day 7)
1-Butanol	-	19	5	4	<2	2
2-Pentanone	-	<2	<2	<2	<2	<2
1-Pentanol	-	2	<2	2*	<2	<2
2-Hexanone	-	2	<2	<2	<2	<2
Hexanal	-	8	3	2	3	2
n-Butyl ether	-	23	<2	<2	<2	2
2-Heptanone	-	10	<2	2	<2	<2
α-Pinene	-	53	3	6	3	4
2-Octanone	-	6	<2	2	<2	<2
3-Carene	-	26	<2	3	<2	2
2-Ethyl-1-Hexanol	-	26	12	8	6	10
Limonene	-	<2	<2	<2*	<2	<2
Material RH (measured)		60-90 %	40-60 %			

[a]Only in one of two samples.

Table 4
VOC compounds from test run with major pressure difference with mineral wool insulation. The column colors (dark grey, light grey, white) indicate the moisture level (relative humidity, RH%) on the sampling day.

	Day 1 (µg/m3)		Day 3 (µg/m3)		Day 6 (µg/m3)		Day 10 (µg/m3)		Day 13 (µg/m3)	
Compound	No mold	Yes mold	No mold	Yes mold	No mold	Yes mold	No mold	Yes mold	No mold	Yes mold
1-Butanol	18	19	6	7	< 2	< 2	< 2	< 2	< 2	-
2-Pentanone	-	228	-	146	3	38	< 2	14	< 2	10
1-Pentanol	13	3	13	3	8	< 2	3	< 2	2	< 2
2-Hexanone	-	55	-	33	< 2	9	-	3	-	2
Hexanal	17	5	11	5	6	< 2	2	< 2	2	< 2
n-Butyl ether	21	13	< 2	< 2	< 2	< 2	-	< 2	-	-
2-Heptanone	2	90	< 2	72	< 2	23	< 2	7	< 2	4
α-Pinene	70	114	127	89	78	33	40	14	13	10
2-Octanone	-	48	-	46	-	23	-	9	-	6
3-Carene	-	116	54	76	72	27	-	12	10	8
2-Ethyl-1-Hexanol	22	20	11	17	8	11	5	9	5	8
Limonene	7	12	7	8	7	3	4	< 2	2	< 2
Material RH (measured)	90-100 %		60-90 %	90-100 %	40-60 %	90-100 %	40-60 %	60-90 %	40-60 %	

[a]Only in one of two samples.

Table 5
VOC compounds from test run with minor pressure difference with mineral wool insulation. The column colors (dark grey, light grey, white) indicate the moisture level (relative humidity, RH%) on the sampling day.

	Day 1 (µg/m3)		Day 3 (µg/m3)		Day 6 (µg/m3)		Day 10 (µg/m3)		Day 13 (µg/m3)	
Compound	No mold	Yes mold	No mold	Yes mold	No mold	Yes mold	No mold	Yes mold	No mold	Yes mold
1-Butanol	19	16	2	3	< 2	-	-	-	-	-
2-Pentanone	-	107	5	75	2	37	-	9	-	4
1-Pentanol	29	3	18	< 2	8	< 2	3	-	2	-
2-Hexanone	-	27	< 2	19	< 2	9	-	< 2	-	-
Hexanal	26	6	15	-	7	2	3	< 2	2	< 2
n-Butyl ether	11	9	< 2	< 2	< 2	-	-	-	-	-
2-Heptanone	3	51	3	32	< 2	22	< 2	5	< 2	2
α-Pinene	36	53	53	42	50	84	6	11	4	8
2-Octanone	-	33	3	26	-	19	-	6	-	3
3-Carene	-	74	28	36	49	82	6	16	5	9
2-Ethyl-1-Hexanol	15	16	6	10	4	7	5	7	5	7
Limonene	4	10	4	6	6	6	< 2	< 2	< 2	< 2
Material RH (measured)	90-100 %						40-60 %			

[a]Only in one of two samples.

wood material or water absorption between single laths. The variation of the material relative humidity in all test runs is presented in Fig. 4.

The relative humidity (RH) of wood material was a bit higher and stayed longer in the laths having mold growth in the cases 1, 3 and 4 where the starting humidity conditions of wooden laths were around the same level. Presence of mineral wool insulation in construction also had impact on the moisture condition of wood material. Wood moisture content stayed longer at higher level during minor and major pressure differences with mineral wool insulation. When no insulation material was used with major pressure difference, the moisture content of studied system seemed to be low compared with the other cases. The final humidity conditions, however, were around the same level within all cases.

The temperature of the test environment was maintained at normal room temperature, and no attempt was made to vary it. Normal room temperature is favorable for microbial growth. Average temperature all test runs varied between 20.8 °C and 23.2 °C. Temporal maximum was 26.7 °C and minimum 18.6 °C.

3.2. Volatile organic compounds

Volatile Organic Compounds (VOCs) were measured from an indoor air chamber using two parallel Tenax TA tubes on days 1, 3, 6, 10, and 13. In the test run with a major pressure difference and no mineral wool insulation, samples were collected only on days 1, 3, and 6 due to the absence of sufficient relative humidity (RH 90–100%), which was not reached. Day 0 was designated as the setup day, and the full duration of each test run was two weeks, except for the test run. Only target compounds were analyzed and are presented in Tables 2–5. The column colors (dark grey, light grey, white) indicate the moisture level (relative humidity, RH%) on the sampling day.

Four compounds—2-pentanone, 2-hexanone, 2-heptanone, and 2-octanone—were clearly associated with microbial growth. These compounds were either absent or present in very low concentrations in the “no mold” test runs, whereas significantly higher concentrations were observed in test runs with active mold growth. The highest

Table 6
Varimax rotated component matrix of principal component analysis of studied compounds. Highly correlated compounds for each PCs ("Component") are bold. The gray background indicates the components selected for each PC.

	Component		
	1	2	3
2-Heptanone	**.974**	.032	.136
2-Pentanone	**.972**	.014	.101
2-Hexanone	**.970**	.018	.170
2-Octanone	**.963**	-.051	.075
Carene	**.561**	**.417**	.273
Hexanal	-.205	**.911**	.136
1-Pentanol	-.191	**.900**	.022
α-Pinene	.239	**.814**	-.026
Limonene	**.533**	**.808**	.035
n-Butyl ether	.035	.036	**.954**
1-Butanol	.184	.145	**.945**
2-Ethyl-1-Hexanol	.212	-.024	**.923**

concentration was observed for 2-pentanone in the following test runs: minor pressure difference without mineral wool (197 μg/m^3), major pressure difference with mineral wool (228 μg/m^3), and minor pressure difference with mineral wool (107 μg/m^3).

Terpene compound concentrations (α-pinene, 3-carene, limonene) varied across all test runs. However, no clear differences were found between mold and no mold conditions, pressure differences, or the presence or absence of mineral wool insulation.

2-Ethyl-1-hexanol concentrations remained low (maximum 22 μg/m^3) across all test setups. In contrast, hexanal and 1-pentanol concentrations were higher in the "no mold" condition (7–44 μg/m^3 and 8–60 μg/m^3, respectively) compared to the mold growth condition (<2–11 μg/m^3 and <2–9 μg/m^3, respectively). No significant differences were observed in the concentrations of 1-butanol and n-butyl ether.

3.3. Principal component analysis

The following variables were included in the component matrix analysis: 1-butanol, 2-pentanone, 1-pentanol, 2-hexanone, hexanal, n-butyl ether, 2-heptanone, α-pinene, 2-octanone, carene, 2-ethyl-1-hexanol, and limonene. The Kaiser-Meyer-Olkin (KMO) Measure of Sampling Adequacy was >0.5, and Bartlett's test of sphericity yielded a p-value <0.0001, confirming the suitability of the data for principal component analysis (PCA). Individual variable communalities ranged from 0.563 to 0.971.

The first three principal components had eigenvalues greater than 1 and accounted for a cumulative variance of 87.91% (PC1: 38.14%, PC2: 26.31%, PC3: 23.46%). These three components were included in the mixed model analysis, while components with eigenvalues below 1 were excluded.

PC1 was strongly correlated with 2-heptanone, 2-pentanone, 2-

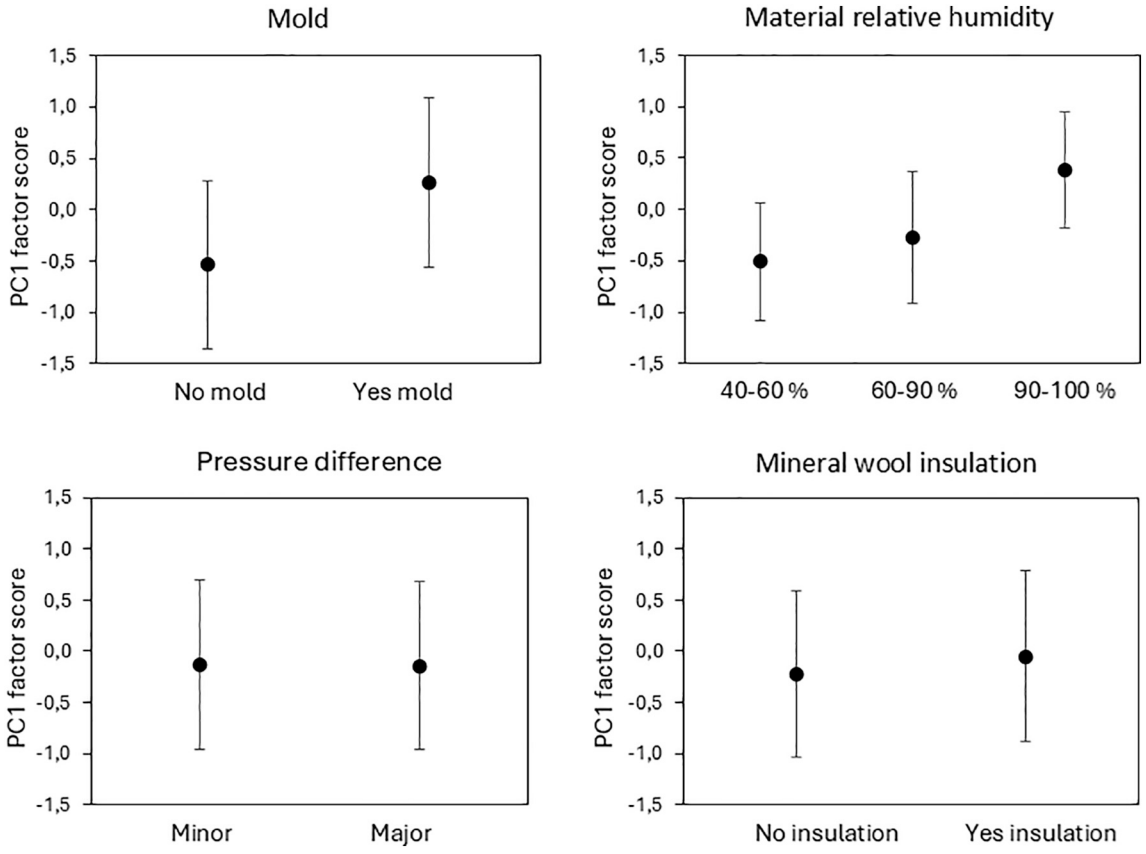

Fig. 5. Principal component 1 (PC1) compared to mold presence (yes/no), material RH (40–60%, 60–90%, 90–100%), pressure difference (minor/major) and insulation presence (yes/no) with 95% confidence limit as error bars.

Table 7
Results of linear mixed model analyses for effect of Mold, RH, dP and Insulation on PCs (PC1: MVOCs, PC2: emissions from wood, PC3: emissions from gypsum board). LCL = lower 95% confidence limit, EMM = estimated marginal mean, UCL = upper 95% confidence limit. RH has three levels thus the pairwise difference between levels was analyzed with Bonferroni post hoc test. Different letters after UCL indicates significant pairwise difference (Bonferroni $P < 0.05$): a = significant between 0 and 1, b = significant between 0 and 2, c = significant between 1 and 2.

Principal component	Variable	LCL – EMM – UCL	Statistics
PC1	Mold	0: (−1.360) – (−0.537) – 0.286 1: (−0.559) – 0.266–1.090	$F_{1,\ 3.827} = 3.738$, $P = 0.129$
	RH	0: (−1.079) – (−0.510) – 0.058 [b] 1: (−0.914) – (−0.276) – 0.362 [c] 2: (−0.189) – 0.380–0.949	$F_{2,\ 59.329} = 11.570$, $P < 0.0001$
	dP	0: (−0.951) – (−0.130) – 0.691 1: (−0.963) – (−0.141) – 0.681	$F_{1,\ 3.944} = 0.001$, $P = 0.981$
	Insulation	0: (−1.035) – (−0.220) – 0.594 1: (−0.886) – (−0.051) – 0.784	$F_{1,\ 3.891} = 0.165$, $P = 0.706$
PC2	Mold	0: (−0.334) – 0.437–1.209 1: (−1.286) – (−0.513) – 0.259	$F_{1,\ 3.987} = 5.791$, $P = 0.074$
	RH	0: (−1.217) – (−0.681) – (−0.146) [a, b] 1: (−0.625) – (−0.030) – 0.565 [c] 2: 0.061–0.597–1.133	$F_{2,\ 59.333} = 27.752$, $P < 0.0001$
	dP	0: (−0.636) – 0.134–0.904 1: (−0.981) – (−0.210) – 0.561	$F_{1,\ 4.095} = 0.750$, $P = 0.434$
	Insulation	0: (−0.647) – 0.118–0.884 1: (−0.976) – (−0.195) – 0.586	$F_{1,\ 4.045} = 0.624$, $P = 0.473$
PC3	Mold	0: (−0.839) – (−0.152) – 0.534 1: (−0.758) – (−0.077) – 0.603	$F_{1,\ 3.758} = 0.047$, $P = 0.840$
	RH	0: (−0.803) – (−0.319) – 0.165 [b] 1: (−1.222) – (−0.584) – 0.054 [c] 2: 0.076–0.559–1.041	$F_{2,\ 60.314} = 10.272$, $P < 0.0001$
	dP	0: (−1.275) – (−0.599) – 0.078 1: (−0.314) – 0.369–1.052	$F_{1,\ 4.044} = 7.641$, $P = 0.050$
	Insulation	0: (−0.843) – (−0.168) – 0.508 1: (−0.762) – (−0.062) – 0.637	$F_{1,\ 3.923} = 0.092$, $P = 0.777$

hexanone, 2-octanone, and carene (loadings between 0.561 and 0.974; Table 6). The first four compounds are ketones commonly associated with microbial volatile organic compounds (MVOCs) from active microbial growth, which was also observed in the present study. Carene, on the other hand, is a terpene typically emitted from wood materials, and PC2 was correlating also with carene.

PC2 was highly correlated with hexanal, 1-pentanol, and the terpenes α-pinene and limonene (loadings between 0.808 and 0.911; Table 6). These compounds are more characteristic of emissions from wood-based materials and, in this study, were found in higher concentrations under "no mold" conditions. PC1 correlates also with limonene.

PC3 was strongly correlated with n-butyl ether, 1-butanol, and 2-ethyl-1-hexanol (loadings between 0.923 and 0.954; Table 6). These compounds were detected at low concentrations and showed minimal variation between "mold" and "no mold" conditions or across different RH levels, suggesting they are primarily emitted from gypsum board.

3.4. Mixed model results

A linear mixed model analysis was conducted to examine the effects of mold presence, material relative humidity (RH), pressure difference, and mineral wool insulation on the principal components derived from VOC measurements. These components represent compressed VOC profiles: PC1 (MVOCs), PC2 (emissions from wood-based materials), and PC3 (emissions from gypsum board). Differences in principal component loadings between categorical variables were further analyzed using the Bonferroni post hoc test.

The presence of mold growth showed no clear statistically significant association with principal component 1 (PC1), representing indoor air concentrations of MVOCs ($F_{1,3.827} = 3.738$, $P = 0.129$), nor with PC3, which reflects emissions from gypsum board materials ($F_{1,3.758} = 0.047$, $P = 0.840$). PC1 shows positive association for mold growth meaning the difference on MVOC concentrations between mold growth and no mold growth (Fig. 5, Table 7). However, a near-significant association was observed between presence of mold and PC2, corresponding to emissions from wooden materials ($F_{1,3.987} = 5.791$, $P = 0.074$). In this case, "mold" had lower PC2 scores compared to "no-mold" (Fig. 6, Table 7), suggesting a possible negative association between mold presence and the level of material-related VOC emissions from wood surfaces. Although this result did not reach conventional statistical significance, it may indicate an underlying pattern that warrants further investigation with larger sample sizes.

Relative humidity (RH) was significantly associated with all three principal components (Figs. 5–7). For PC1, representing MVOCs, RH had a strong effect ($F_{2,59.329} = 11.570$, $P < 0.0001$), with higher RH levels corresponding to higher PC1 scores. Similarly, RH showed a highly significant association with PC2, reflecting emissions from wood-based materials ($F_{2,59.333} = 27.752$, $P < 0.0001$), and with PC3, related to emissions from gypsum board ($F_{2,60.314} = 10.272$, $P < 0.0001$). These results suggest that material increased relative humidity is consistently associated with elevated levels of various indoor air compounds, possibly due to enhanced off-gassing or microbial activity at higher moisture levels. Differences and confidence intervals across RH levels further indicate clear and systematic trends in VOC profiles linked to material relative humidity.

Air pressure difference (dP) over the wall structure showed no statistically significant association with PC1 ($F_{1,3.944} = 0.001$, $P = 0.981$) or PC2 ($F_{1,4.095} = 0.750$, $P = 0.434$), suggesting that pressure-driven air infiltration may not substantially influence MVOC levels or emissions from wooden materials in this dataset. However, a borderline significant association was observed for PC3, related to gypsum board emissions ($F_{1,4.044} = 7.641$, $P = 0.050$). In this case, higher pressure differences corresponded to higher PC3 scores, potentially indicating that pressure-driven air movement could influence the release or redistribution of certain VOCs originating from building materials such as gypsum board.

No statistically significant effects of insulation status were found for any of the principal components. For PC1 (MVOCs), the effect of insulation was non-significant ($F_{1,3.891} = 0.165$, $P = 0.706$), as was the case for PC2 (wood material emissions; $F_{1,4.045} = 0.624$, $P = 0.473$), and PC3 (gypsum board emissions; $F_{1,3.923} = 0.092$, $P = 0.777$). These results suggest that insulation presence or absence, as defined in the current model, does not have a measurable influence on the indoor air chemical profiles represented by the PCA components. This may reflect either a true lack of effect or limitations in how insulation characteristics were categorized or captured.

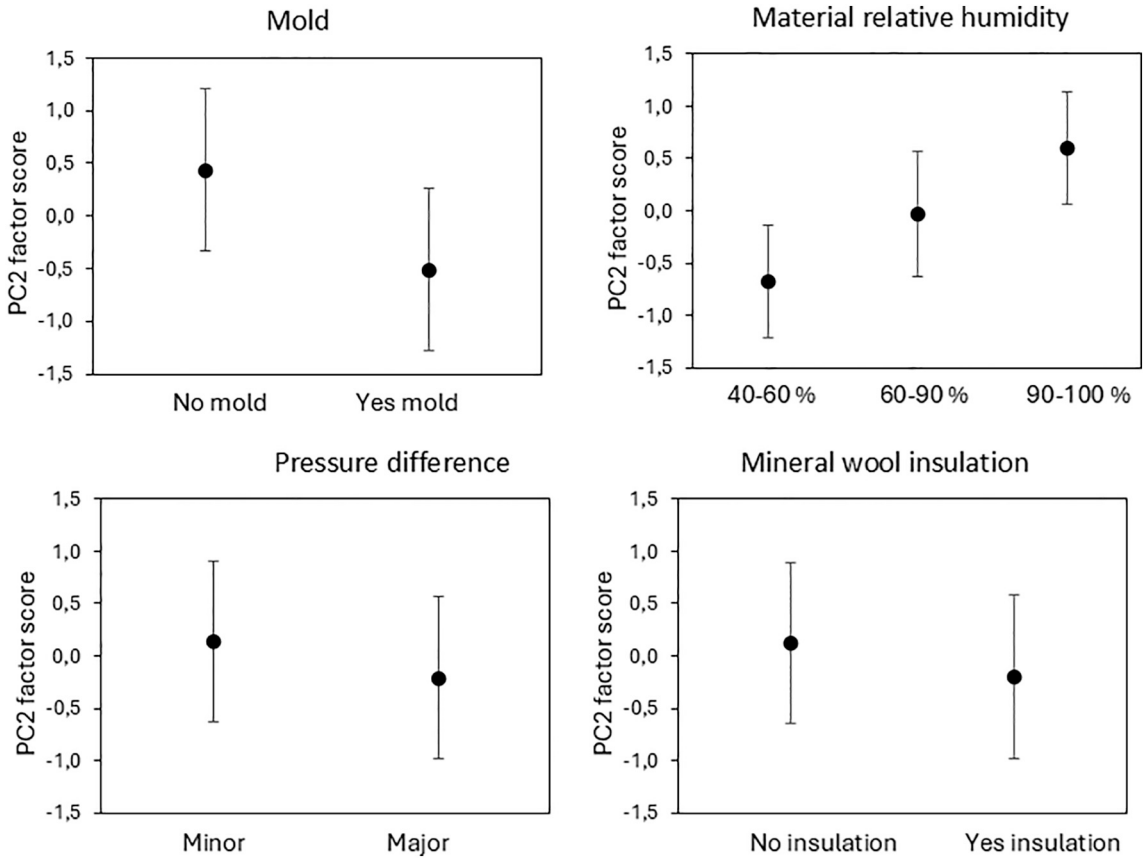

Fig. 6. Principal component 2 (PC2) compared to mold presence(yes/no), material RH (40–60%, 60–90%, 90–100%), pressure difference (minor/major) and insulation presence (yes/no) with 95% confidence limit as error bars.

3.5. Limitations

Several limitations should be acknowledged when interpreting the results of this study. The sample size was relatively small, particularly in some subgroup comparisons (e.g., mold presence or insulation status), which limited statistical power. This is reflected in some near-significant findings that may have reached significance with a larger dataset. Although principal component analysis (PCA) effectively reduced dimensionality and grouped correlated VOCs, the interpretation of components remains somewhat abstract and dependent on the selected input variables. As such, linking principal components directly to specific sources should be done cautiously. Also, the presence or absence of mold and insulation were treated as binary variables, potentially oversimplifying complex conditions. More nuanced or quantitative assessments (e.g., mold area, spore counts, insulation thickness or material) would likely offer greater explanatory power. Finally, the observational nature of the data limits causal inference: while associations can be identified, the direction and mechanisms of influence cannot be conclusively established.

4. Discussion

The aim of this study was to find the most critical factors from an air leakage moisture damaged wall structure into indoor environment utilizing multivariate methods and principal component analysis. Simulation test runs carried out in a steady laboratory environment (IAQ simulator). The impact of wood material relative humidity changes with and without mold growth on VOC emissions were evaluated under minor and major pressure difference between indoor and outdoor air chambers. Also, the effect of mineral wool insulation material was studied. All test runs carried out with new materials, however, each wall structure (wood material) behaved individually even wood materials were stored in constant circumstances and water was added as much for each test run. For this reason, relative humidity varied a little unexpectedly during test runs and all moisture levels did not reach one of the setups. The relative humidity of the wood material was measured simultaneously with the VOC sample. The same tests were performed on wood material with and without microbial growth. The VOC results were classified based on the relative humidity of the measured material. In this case, the results specifically indicate the effect of the moisture conditions on VOCs.

VOCs measured from indoor air chamber with two parallel samples on test days. Four compounds (2-pentanone, 2-hexanone, 2-heptanone, and 2-octanone) were clearly found originated from microbial growth as shown also in previous studies (Claeson, 2006, Korpi et al., 2009, Pasanen et al., 1997, Schleibinger et al., 2005). These compounds were not or were on very low concentrations in “no mold” test runs, while in test runs with active mold growth concentrations of these compounds were much higher. The highest concentration was 2-pentanone in test runs minor pressure difference without wool, major pressure difference with wool, and minor pressure difference with wool 197, 228, and 107 µg/m3, respectively. However, concentrations decreased rapidly together with moisture level.

Terpene compound concentrations (α-pinene, 3-carene, limonene) varied during all test runs, however, a clear difference between cases mold and no mold, major and minor pressure difference, or with and without wool insulation did not find. 2-ethyl-1-hexanol concentrations were low (maximum 22 µg/m3) in all test setups. Hexanal and 1-pentanol concentrations were higher in case with no mold (7–44 µg/m3 and 8–60 µg/m3) compared to case with mold growth (<2–11 µg/m3, <2–9 µg/m3), respectively. 1-butanol and n-butyl ether concentrations did not find differences. These compounds are not generally identified as

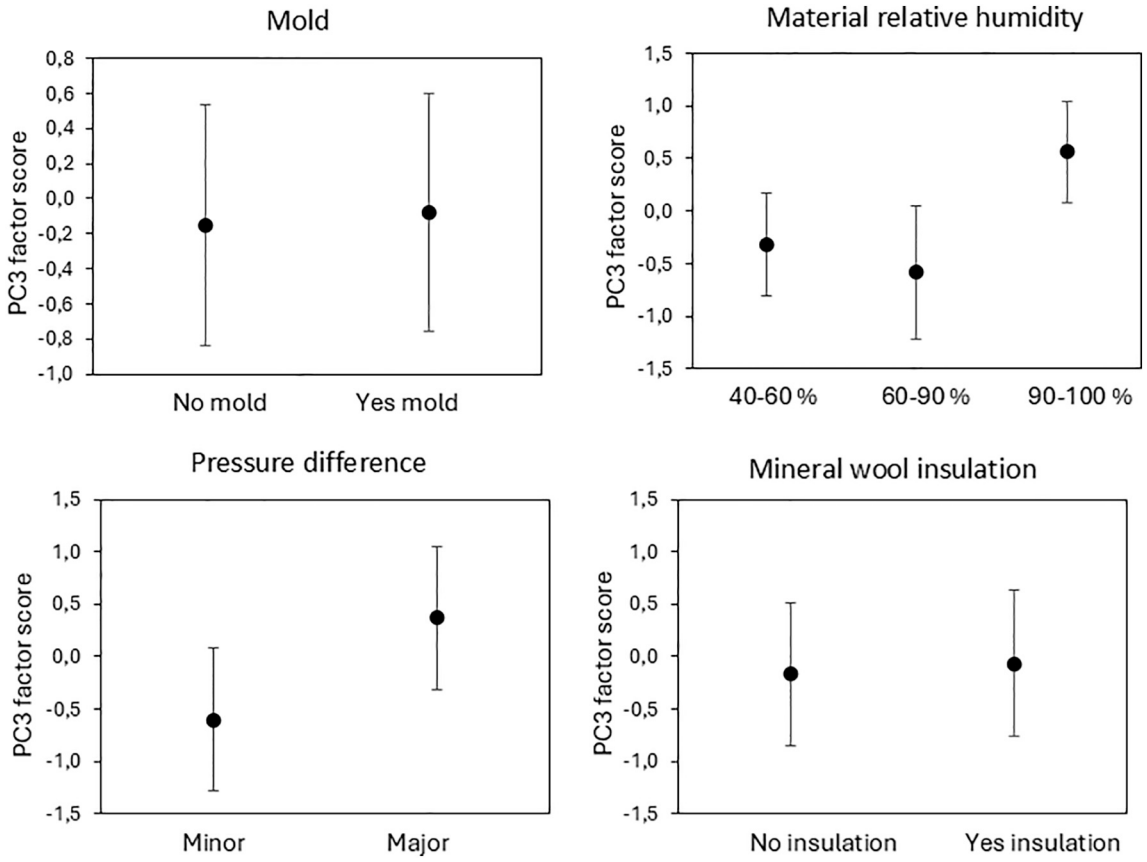

Fig. 7. Principal component 3 (PC3) compared to mold presence(yes/no), material RH (40–60%, 60–90%, 90–100%), pressure difference (minor/major) and insulation presence (yes/no) with 95% confidence limit as error bars.

MVOCs, however, these may emit from moisture damaged materials. Only wood, gypsum board and mineral wool were used in this study when VOC emission can be linked to these materials. In a real building, there are many more emission sources.

The present analysis revealed varying associations between building-related variables and indoor air chemical profiles as represented by the three principal components. Mold growth was not significantly associated with PC1 (MVOCs) or PC3 (gypsum board emissions) but showed a near-significant negative association with PC2, which reflects emissions from wooden materials. The presence of mold growth had lower PC2 scores, suggesting that microbial contamination may interact with or suppress certain VOC emissions from wood surfaces. Although not statistically significant at the conventional 0.05 level, the observed trend warrants further exploration.

Relative humidity (RH) showed consistent and strong associations with all three components. Higher RH was linked to elevated levels of ketones and carene (PC1), emissions from wood materials (PC2), and emissions from gypsum board (PC3). These findings suggest that increased humidity may enhance the release of VOCs from various material sources, potentially through moisture-driven diffusion or microbial activity. However, all test runs did not exceed the highest RH level which may have affected the comprehensiveness of the results. The systematic influence of RH across chemical groups underscores its importance as a key environmental determinant in indoor air quality. Terpene, aldehyde, organic acids, and alcohol emissions from wood material in different indoor air RH conditions studied also in Sivula et al. (2025) where main emitted compounds were α-pinene and 3-carene from terpenes and hexanal from aldehydes. Both, terpenes and aldehydes, were dependent both indoor air RH and time (Sivula et al., 2025).

Pressure difference (dP) had no significant effect on PC1 or PC2, but a borderline association with PC3 suggests that pressure-driven airflow may influence VOC transport, particularly those originating from gypsum board surfaces. However, due to the marginal significance level and small degrees of freedom, this result should be interpreted with caution. It is notable that airflow was higher in lower pressure difference case what makes this variable difficult to analyze. This phenomenon is known in existing buildings where the importance of air leakage needs to be assessed. When there are a lot of air leakage routes in structures, it may be even impossible to reach high pressure difference. However, the airflow may be higher compared to major pressure difference what has been considered less acceptable. Further studies with controlled pressure conditions are recommended to clarify this relationship.

Insulation status did not show any statistically significant associations with the principal components. The lack of observed effects may reflect a true absence of impact, or limitations in the resolution or categorization of insulation characteristics in the current dataset. Future studies could benefit from more detailed metrics of insulation type, thickness, and installation quality to better assess its role in VOC and airflow dynamics.

The purpose of PCA in this study was to reduce data complexity by transforming numerous correlated VOC measurements into a smaller set of uncorrelated principal components (PCs) that capture most of the variance. Each PC represents a group of compounds with similar environmental origins, such as microbial growth (MVOCs), wood-based materials, or gypsum board. This classification is justified because these groups reflect underlying sources rather than individual compounds, enabling more meaningful interpretation of exposure patterns. Instead of analyzing mold, relative humidity, pressure difference, and insulation effects on each VOC separately, we assessed their influence on these composite indicators.

The measurements and procedures in this study were conducted in accordance with the ISO standards that were valid at the time of data

collection (ISO, 2004; ISO, 2006). Since then, several of these standards have been revised or updated (ISO, 2021). While the methodology used reflects the best practices available at the time, readers should note that newer versions of the relevant ISO standards may contain updated requirements, definitions, or measurement techniques. These changes may influence comparability with future studies or current regulatory interpretations. However, the core principles of the applied standards remain consistent, supporting the validity and relevance of the collected data within the context of the original study framework.

5. Conclusions

The key conclusions of the study demonstrated that material relative humidity (RH) was overwhelmingly the most significant single factor influencing the levels of all identified VOC concentrations; higher humidity consistently led to elevated emissions. Specifically, four ketones were clearly identified as originating from microbial growth, and the presence of active mold growth was determining factor. However, presence of mold growth showed a weak negative association with VOC emissions from wood materials, potentially indicating a complex interaction between microbes and material emissions. The mineral wool insulation had no statistically significant impact on any of the investigated VOCs.

Air pressure differential exhibited only a borderline significant effect. As the pressure difference in the test environment was controlled by adjusting the number of air leakage pathways, it was observed that the highest volumetric airflow due to leakage occurred under conditions with a lower pressure difference. This phenomenon is also commonly observed in real buildings. The airtightness of a building influences the pressure differential across the building envelope. For example, in buildings with poor airtightness, large pressure differences between indoor and outdoor air are less likely to develop, yet the total amount of air leakage can still be substantial.

Multivariate methods like PCA are established statistical techniques that identify latent structures by exploiting correlations among variables. They reduce dimensionality while preserving key information, improving interpretability in complex datasets. Although widely used in other fields, their application indoor air research is still rare. In this context, PCA provides a robust framework for understanding source-related patterns in VOC profiles and offers a valuable tool for indoor air investigations.

CRediT authorship contribution statement

V. Lappalainen: Writing – original draft, Visualization, Methodology, Investigation. **J. Sorvari:** Writing – review & editing, Methodology, Data curation. **E. Sohlberg:** Writing – review & editing, Methodology, Investigation. **P. Pasanen:** Writing – review & editing, Validation, Supervision, Conceptualization.

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work the authors used Copilot (Microsoft) to improve the readability and language of the manuscript. After using this tool, the authors reviewed and edited the content as needed and took full responsibility for the content of the published article.

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Declaration of competing interest

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Data availability

Data will be made available on request.

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