All the airflow models with the Eulerian method predicted reasonable results, but failed to reproduce a high concentration zone at the lower-right corner. The performances of different airflow models were similar. This is because all the models shared the same scalar transport equation.

All the airflow models with the Lagrangian method predicted similar distributions except the URANS model, which predicted a larger high concentration zone on the left side of the room. The results from the Lagrangian method were more scattered than those from the Eulerian method due to its discrete nature. This phenomenon was also reported by several other studies [7, 10]. The results from the LES, DES1, and DES2 were even more scattered than those from RANS and URANS. This is understandable since the LES and DES models reproduced more unsteady eddy structures, which contributed to the turbulence dispersion of the particles. In contrast, the RANS and URANS used the isotropic DRW model to account for the turbulence dispersion, which led to a more diffusive particle concentration pattern.

3.2. Particle dispersion in a room with displacement ventilation

In the previous case, the ventilation rate was very high for an enclosed environment, and the case was isothermal. Therefore, this investigation chose a non-isothermal test case with a lower ventilation rate, as shown in Figure 3. The room had a UFAD system and four heated boxes simulating occupants. The air supplied from the two floor openings had a total flow rate of 0.0994 m^3/s, and it was exhausted from the ceiling. Monodispersed particles with a diameter of 0.7 μm were released into the room from a point source at 0.3 m above the floor. Note that indoor particles of this size are in the accumulation mode, which have low deposition rate [6]. Therefore, the particle deposition and gravitational sedimentation were neglected in the numerical simulation. The particle concentration was measured at six poles in the room, as shown in Figure 4. A more detailed description of the experiment and boundary conditions can be found in reference [6].

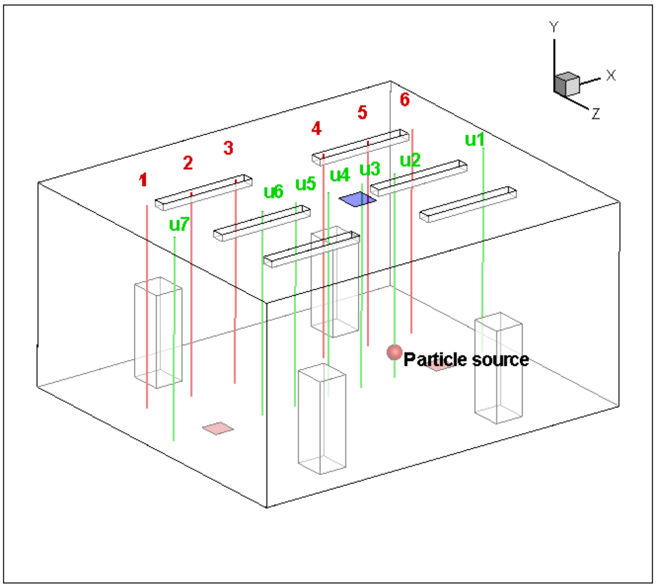

Figure 4 Schematic view of the non-isothermal room in which the particle concentration was measured at different heights along the six red lines, and air velocity was measured at the seven green lines

This CFD study again tested three grid resolutions (44,100, 352,100, and 1,630,000) to simulate the flow. The 352,100 grids generated similar results to those of the 1,630,000 grids; the results from the 352,100 grid are reported in this paper. The RANS-Lagrangian model used 500,000 trajectories. For the unsteady airflow models (URANS, LES, and DES1, and DES2) with the Lagrangian method, the particle generation rate was 1,000 particles per second. The transient concentration fields were averaged over ten minutes, corresponding to on complete air change. For the unsteady airflow models with the Eulerian method, the scalar concentration fields were also averaged over ten minutes. Again, the time step used in this case was 0.01s.

Figure 5 compares the simulated and measured air velocity at seven different poles (green lines in Figure 4). In general, the five turbulence models predicted comparable results for the air velocity, while the RANS model slightly over-predicted air velocity at the lower part of pole u1 and u2. At pole u7, all the five turbulence models over-predicted air velocity at lower part of the room.

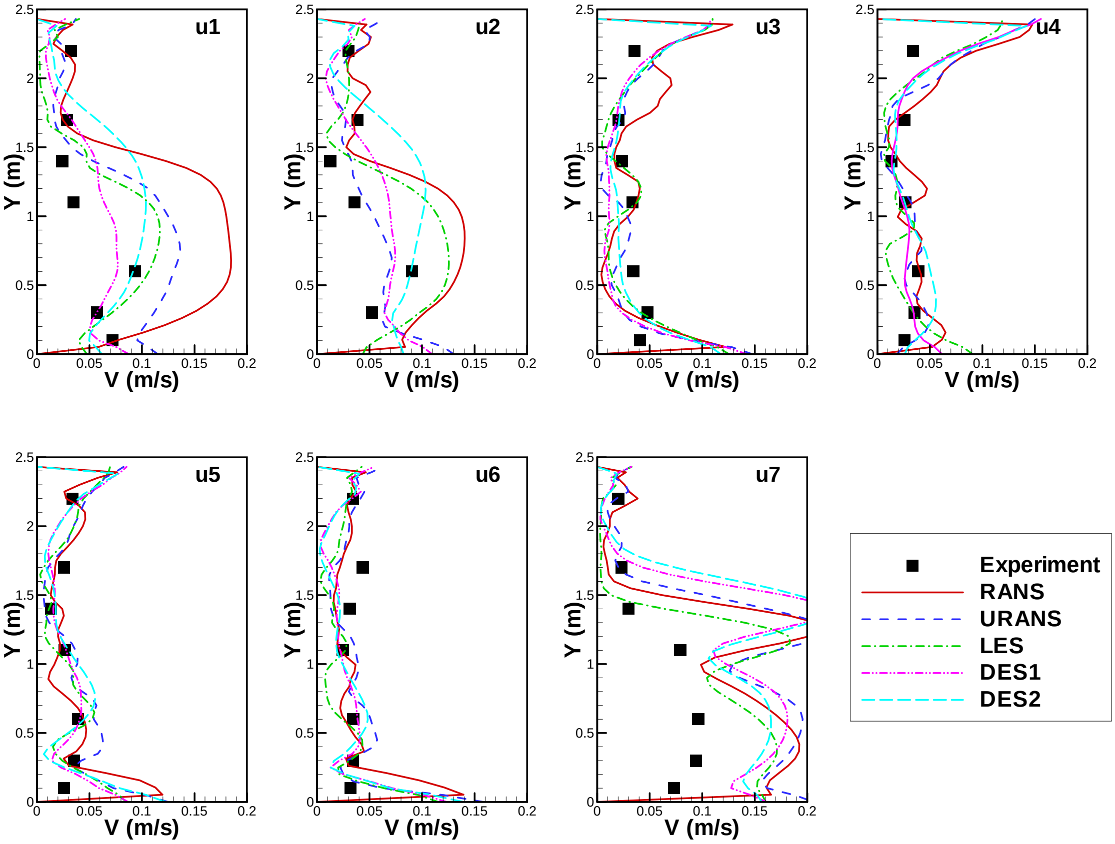

Figure 5 Comparison of the simulated and the measured air velocity at seven poles in the room with displacement ventilation.

Figure 6 compares the particle concentration profiles calculated by the five airflow models with the Eulerian method. As in the previous case, all the models predicted comparable results with correct magnitude. The URANS model over-predicted the concentration at the lower part of poles 2 and 3. The DES2 model under-predicted the concentration at the lower part of poles 3 and 4. The LES and two DES models predicted a straight profile at pole 5, while RANS and URANS predicted slightly better results. All the models predicted a straight profile at pole 6, where the experiment showed a higher concentration near the ceiling and floor than in the middle.

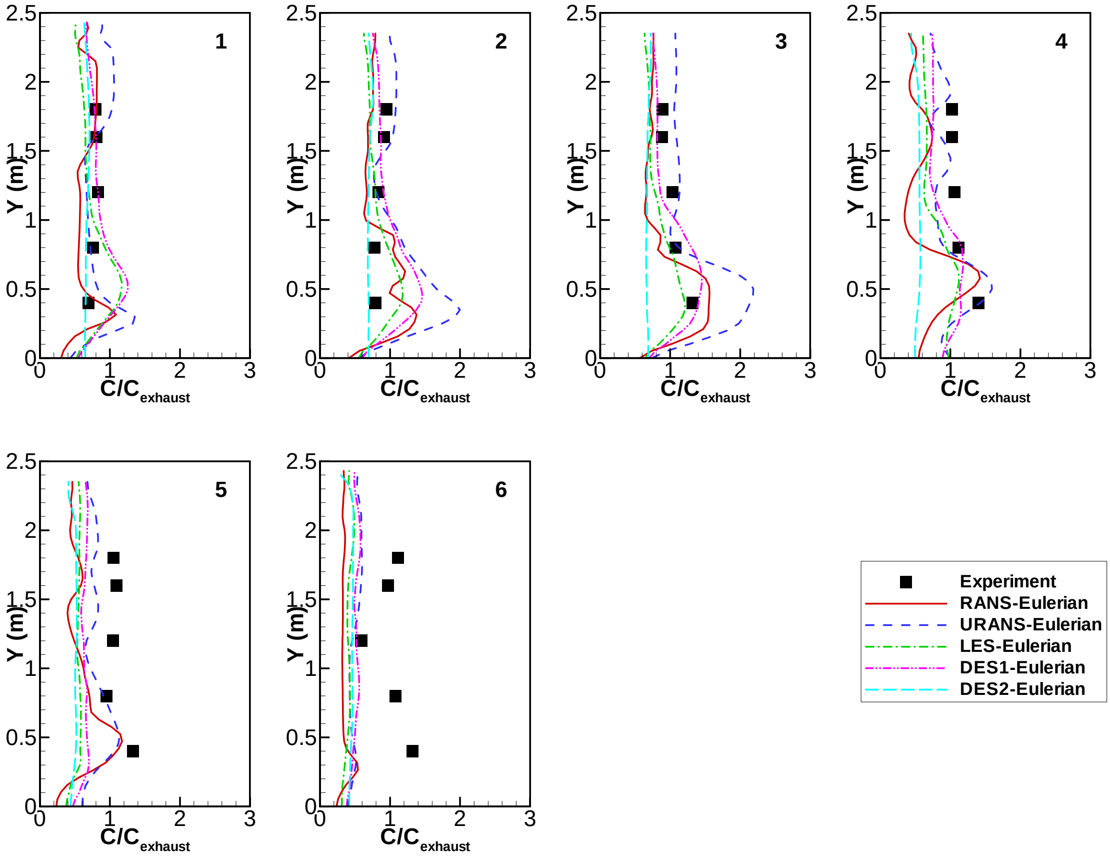

Figure 6 Comparison of the measured and calculated particle concentration profiles with the Eulerian method at the six poles in the room with displacement ventilation.

Figure 7 compares the particle concentration profiles calculated by the five airflow models with the Lagrangian method. Again, the results from the Lagrangian method were more scattered than those of the Eulerian method. Unlike the Eulerian method, the five models with the Lagrangian method showed a quite different performance. The URANS model and RANS model predicted large fluctuations at poles 2, 3, and 4. This was because, at these locations, the airflow driven by mechanical ventilation interacted with the thermal plumes, which generated an unstable separated flow. The RANS and URANS models could not perform well for such flow features [11]. In contrast, the LES and DES predicted more realistic profiles due to the better performance of an unstable flow.

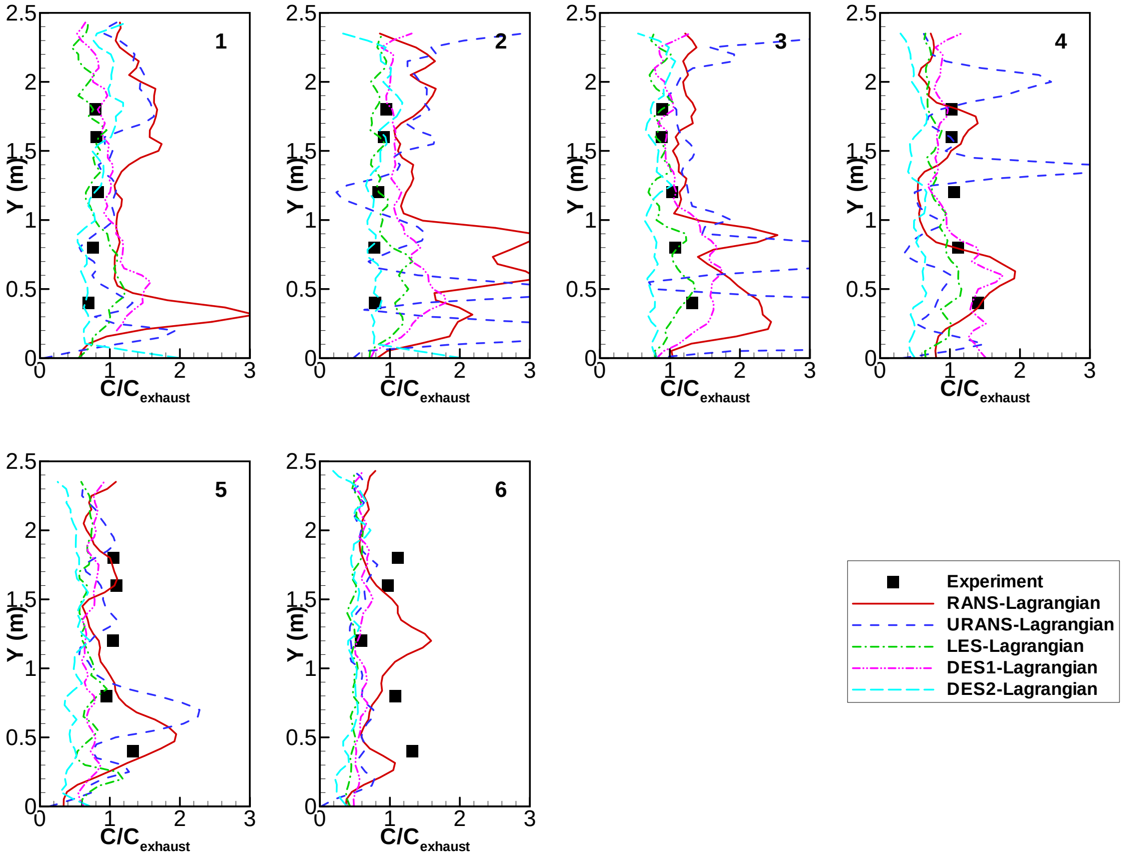

Figure 7 Comparison of the measured and calculated particle concentration profiles with the Lagrangian method at the six poles in the room with displacement ventilation.

3.3. Transient particle dispersion in a two-zone chamber

In the previous two cases, the contaminant source and the flow field were in steady state. The particle concentration field did not vary with time, which may not be the case in real enclosed environments. However, due to the complexity in measuring transient particle concentration, unsteady particle dispersion processes have not been well studied. Among the few transient particle dispersion experiments in the literature, the case measured by Lu et al. [24] was one of the best. As shown in Figure 8, a three-dimensional two-zone chamber was connected by a sliding door, which could be either fully open or closed. The ventilated air was supplied to the left zone (zone 1) through an opening located on the wall near the ceiling. In the right zone (zone 2), the air was exhausted from another opening near the floor. The air change rate was 10.26 ACH. The particle concentration was measured by an infra-red particle monitor at the center of each zone.

Initially, the sliding door was closed and the ventilation system was turned off. Particles of five size groups (1, 2, 3, 4 and 5 μm) were released into zone 1 and mixed with the room air until uniformly distributed. When the experiment began, the sliding door was opened, and the ventilation system was turned on. The particle concentrations at the center of each zone were measured every minute for a total of 26 minutes. In this case, the rate of particle deposition was one order magnitude smaller than the particle extract by the ventilation system [24]. Therefore, this study neglected the influence of particle deposition.

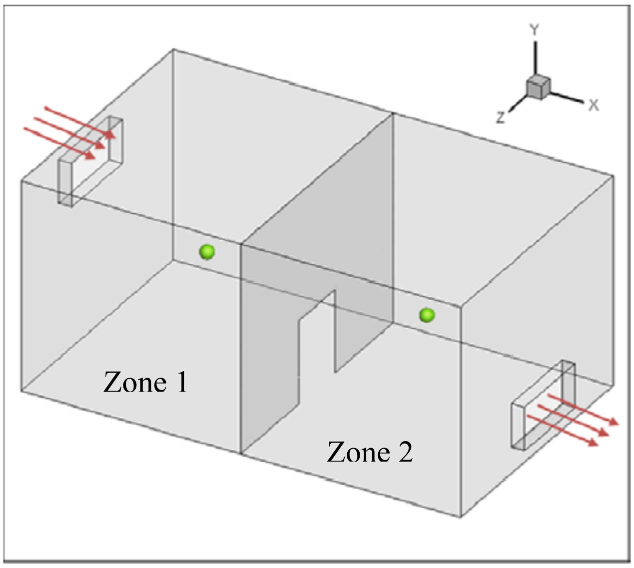

Figure 8 Schematic view of the two-zone chamber in which particle concentration was measured at the centers of the two zones.

Our investigation simulated this case from 0 to 26 minutes with a time step size of 0.01s. Three grid resolutions (26,600, 273,160, and 983,360) were tested for CFD grid independence. The 273,160 grid was sufficiently fine to capture such a flow and was used in particle tracking. Initially, one million particles were randomly located in zone 1, which was tested to be uniformly well distributed. Due to the unsteady nature of this case, only the transient solution was studied, and the steady RANS model was not used for this case. Note that the airflow field measurement was not available for this case. Therefore, the predicted airflow field was compared with the measurement.

Figure 9 shows the particle concentration evolution in the two zones predicted by different models. In zone 1 (Figure 9 (a) and (b)), the particle concentration decayed with time. The Eulerian model predicted decay profiles with too high concentration using the URANS model. This was because the URANS model could not capture the characters of the rapidly changing flow. The two particle models performed reasonably well with LES, DES1, and DES2 models, while the two DES models predicted slightly better results than did LES in terms of magnitude. For all flow models, the Lagrangian method predicted a small fluctuation after 15 minutes when the particle concentration was low. The Eulerian method predicted a smooth profile due to its scalar nature.

In zone 2 (Figure 9 (c) and (d)), again, the URANS model predicted incorrect results using both the Eulerian and Lagrangian methods. The LES, DES1, and DES2 models showed comparable performances. The Eulerian method predicted a larger fluctuation in the first six minutes, while the Lagrangian method predicted better results since it accounted for more physics of flow and particle motion. After 20 minutes, all the models over-predicted the particle concentration, which was also reported by Lu et al. [24].

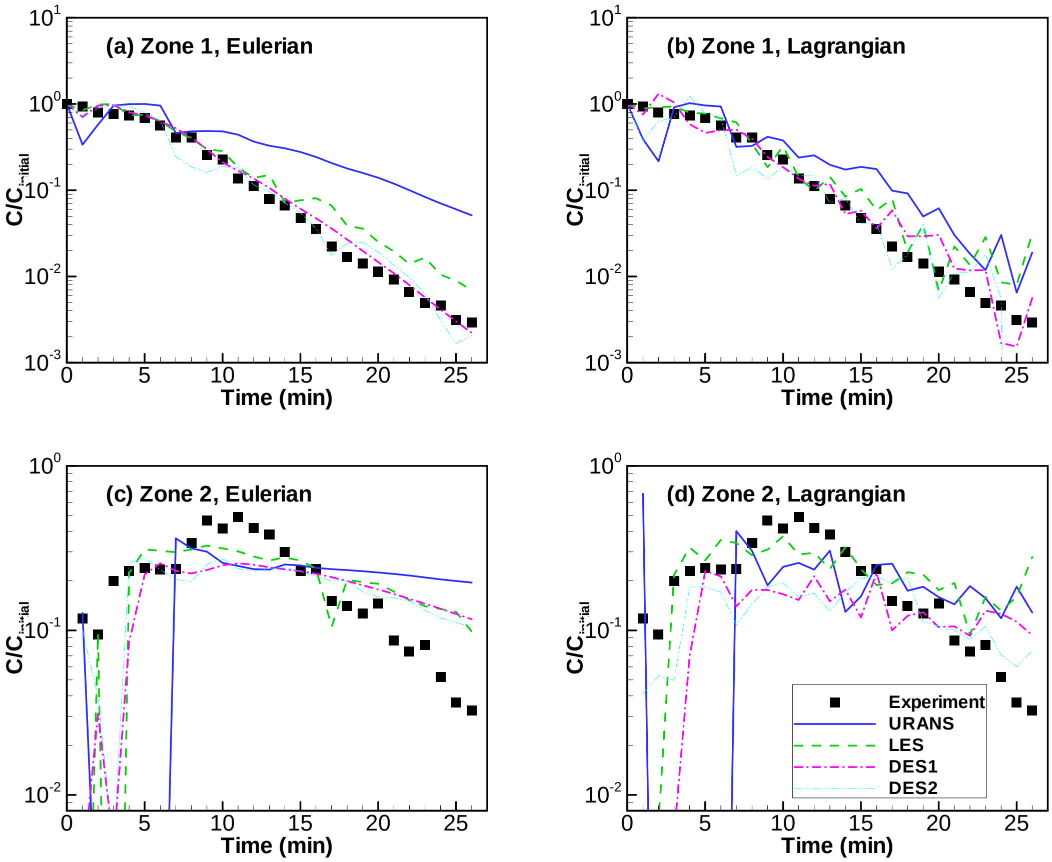

Figure 9 Comparison of the measured and predicted particle-concentration evolution in the two-zone chamber.

4. Discussion

While this investigation tested five airflow models with the Eulerian and Lagrangian methods for the three ventilation cases, it is of great interest to find out how to choose a model for a particular scenario. Table 1 summarizes the applicability and computing cost of each model. For the steady-state case, the Eulerian method can be applied with all five airflow models. The transport equation of the Eulerian method was identical for all airflow models. The resolved airflow was not the main factor in determining the particle distributions. For the Lagrangian method, the particle distribution pattern was primarily determined by the accuracy and richness of the flow structure resolved by the airflow model. Therefore, in many engineering flows with complex flow features, the isotropic RANS and URANS models tested in this study did not work well with the Lagrangian method. The performance may be improved if an anisotropic RANS model is applied. A LES or DES model is needed to provide well-resolved eddy structures for particle tracking.

Besides the accuracy, the computing cost is another important aspect in selecting models. For steady-state flows, the RANS model with the Eulerian method is the most cost efficient. However, if more detailed information is needed or particle dispersion is very complicated, such as chemical reaction, particle deposition, coagulation, and heat and mass transfer, the Lagrangian method should be used with a LES or DES model.

Table 1 Applicability and computing costs of different particle simulation models.

Method		**Steady-state flows**	**Unsteady-state flows**	**Computing time (hour)***		
				Case 1	**Case 2**	**Case 3**
Eulerian	RANS	Yes	No	1.0	3.7	N/A
	URANS	Yes	No	15.4	74.2	62.2
	LES	Yes	No	28.8	75.0	323.3
	DES1	Yes	No	29.2	73.3	367.0
	DES2	Yes	No	34.1	98.3	396.6
Lagrangian	RANS	No	No	2.4	5.3	N/A
	URANS	No	No	17.9	81.5	84.9
	LES	Yes	Plausible	32.4	93.3	360.5
	DES1	Yes	Plausible	33.1	83.3	389.2
	DES2	Yes	Plausible	39.1	118.3	434.3

* The computing time was estimated on an eight-core cluster, with two 2.5GHz AMD quad-core processors and 32GB of memory.

For many unsteady-state cases, the URANS model failed to predict correct transient airflow [21]; thus, it should not be used. With the LES, DES1, and DES2 models, the Eulerian and Lagrangian methods showed a similar performance when the flow was in steady-state and the particle concentration field was in unsteady-state. However, when the flow field is still developing, the Lagrangian method may have better accuracy than the Eulerian method since it accounts for more physics of flow and particle motion. This conclusion is supported by Zhang and Chen [6], who simulated a cough case using both Eulerian and Lagrangian methods. They found that the Eulerian method generated unrealistic results.

5. Conclusions

This study compared the performance of five airflow models with the Eulerian and Lagrangian methods in predicting particle concentration distributions in enclosed environments. The five airflow models were a RANS model, a URANS model, a LES model, and two DES models. The study tested these models for two steady-state particle dispersion cases, a forced convection in a clean room and a mixed convection in a room with a UFAD system, as well as for an unsteady-state case, a ventilated two-zone chamber. The test results showed that the Eulerian method performed in a similar way for all five airflow models. The Lagrangian method predicted an incorrect particle concentration profile with the RANS and URANS models, but did well with the LES and DES models.

For steady-state cases, the RANS model with the Eulerian method is preferred for their reasonable accuracy and low computing cost. For unsteady-state cases, the LES or DES models with the Lagrangian method should be applied, in spite of the high computing cost. The Eulerian method may be improved if take into account more physics, such as gravitational force, Brownian motion and particle deposition.

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