Supporting Materials

Manuscript: **Can a stepwise steady flow CFD model reproduce unsteady PM separation for common unit operations?**

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Pages: 9

Figures:

Figure S1. Frequency distributions of influent flow for monitored events for VCF, HS and PC.

Figure S2. Monitored influent and effluent PSDs for runoff events for VCF, HS and PC. Range bars represent the range of the monitored PM (% finer by mass) for each particle size of the PSD.

Figure S3. Plots illustrating the factor for additional surface area (SA) required as a function of model error (as RMSE) for the VCF, PC and HS in order to reproduce the measured PM separation (ΣE_{PM}). The dashed lines represent one standard deviation of PM separation from monitored data. The HS is loaded by one of the two parallel and identical 544 m^2 catchments of the paved watershed.

Figure S4. Stepwise steady flow error for event-based PM mass as a function of event peak flow.

Figure S5. Stepwise steady flow model error as a function of increasing discretization of unsteady loadings into steady flow steps. Results are illustrated for the VCF for 29 April 2006 and the PC and for the HS for 30 June 2005 storms, respectively. Computational time as a function of increasing discretization of unsteady loadings into steady flow steps is illustrated.

Frequency distribution of flows

All of the events monitored and modeled are unsteady with varying degrees of unsteadiness and differing magnitudes of peak flow. Figure S1 summarizes the normalized frequency distributions (f_n) of flow rates based on normalizing each monitored flow rate to the monitored peak flow experienced by each unit operation over the monitoring campaign. Each unit operations was designed and sized based on the contributing watershed area, noting that the HS of 0.63 m^2 overflow surface area was loaded by only one of the two parallel and identical bridge deck catchments (each 544 m^2, one eastbound and one westbound).

Influent and effluent particle size distributions (PSD)

Figure S2 summarizes the median influent and effluent PSDs across runoff events monitored for the VCF, PC and HS as a mass-based cumulative PSD. While all influent and effluent PSDs are heterodisperse, effluent PSDs are less heterodisperse with the sediment fraction (> 75 μm) largely separated by the VCF and PC. Range bars for each PM size (d_p) represent the mass fraction that each PM size represents across events monitored for each unit operation.

The role of modeling error on sizing design of the unit operations

The stepwise steady and the fully unsteady CFD models are representations of monitored PM separation behavior for each unit operation. RMSE and RPD are utilized to quantify differences between each CFD modeling methods and measured PM separation. Since the PM separation is a function of the unit's appropriate form of surface area (SA), surface area is utilized as a primary design parameter as a unit sizing criterion that is impacted by model error. For the HS and PC the appropriate form of SA is the actual surface overflow area of each unit combined with Newton's Law for discrete Type I particle settling which is appropriate given the coarser, heterodisperse PSD loadings and residence times that are nominally less than an hour in each unit and at some flows on the order of several minutes. For the VCF the appropriate form of SA is the radial SA of the filter for surface loading rate determination. The radial filters control the PM separation behavior of the VCF at a given surface loading rate. For each unit operation of known surface area (tabulated in Figure S3) the analysis utilizes the mean and standard deviation of PM separation from each unit determined from the monitoring campaign. Since the error generated by CFD modeling expresses the difference in PM separation from the known PM separation this difference is used to determine the additional surface area required. This surface area is presented as a factor of the actual monitored unit SA (factor of 1) as shown in Figure S3.

Range and scatter of stepwise steady flow modeling errors for each unit

Figure S4 depicts the event-based stepwise steady flow RMSE for PM separation as a function of increasing peak influent flow rate. The magnitude and range of error is progressively larger for the PC and HS compared to the VCF as peak flow rate increases.

Measurement of PSDs

The measured PSD resolution ranges from 0.02 to 2000 μm, in 100 logarithmic size increments. The discretization is performed on a logarithmic scale. It is also noted that this resolution is that of the Mie scattering based[1] laser diffraction particle size analyzer (Malvern Mastersizer 2000).

The role of discretization on stepwise steady model performance and computational time

Figures 4 and 5 illustrate unsteady and stepwise steady CFD model results in comparison to measured results with model results generated at each monitoring point (for PSD and PM). In an additional analysis the discretization steps for the stepwise steady flow model are further increased by interpolating PSD results and utilizing flow rates between monitoring points of PSDs. Results are illustrated for the 29 April 2006 and 30 June 2005 event with 18 and 16 monitoring points respectively for PSDs, and these monitoring point discretization steps are extended up to 36 discretization steps in Figure S5. Results illustrate an asymptotic limit for reducing model error of 7 (VCF) to 12 (HS) discretization steps for a stepwise steady CFD model. At the same time computational time is additive since each discretization step requires independent continuous phase and discrete phase resolution by the CFD model.

Supplemental references

[1] Finlayson-Pitts, B.J; Pitts, J.N. *Chemistry of the Upper and Lower Atmosphere – Theory, Experiments and Applications*, 1st Ed.; Academic Press: CA, USA, **2000**, 365-368.

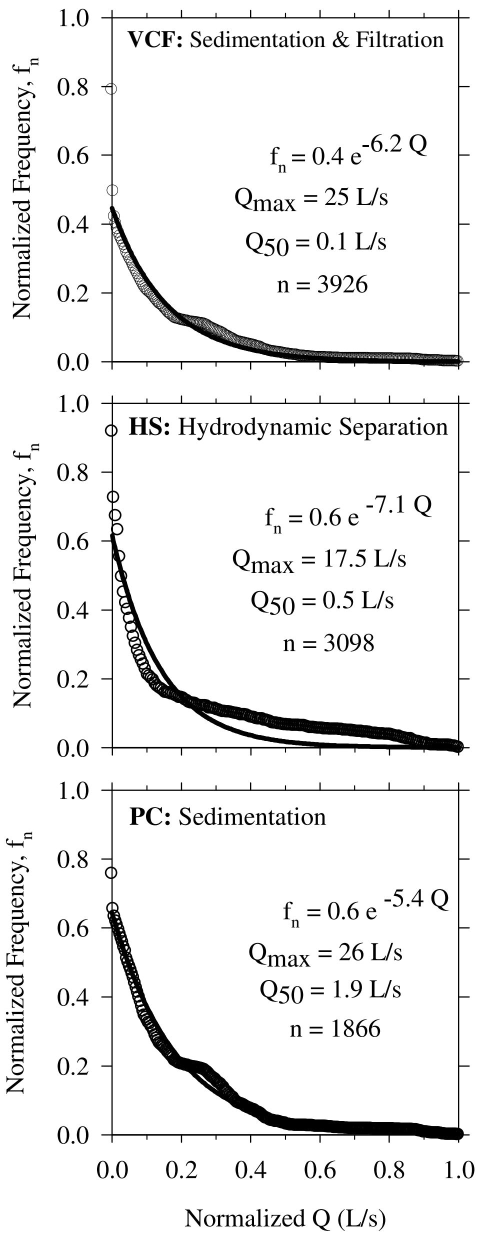
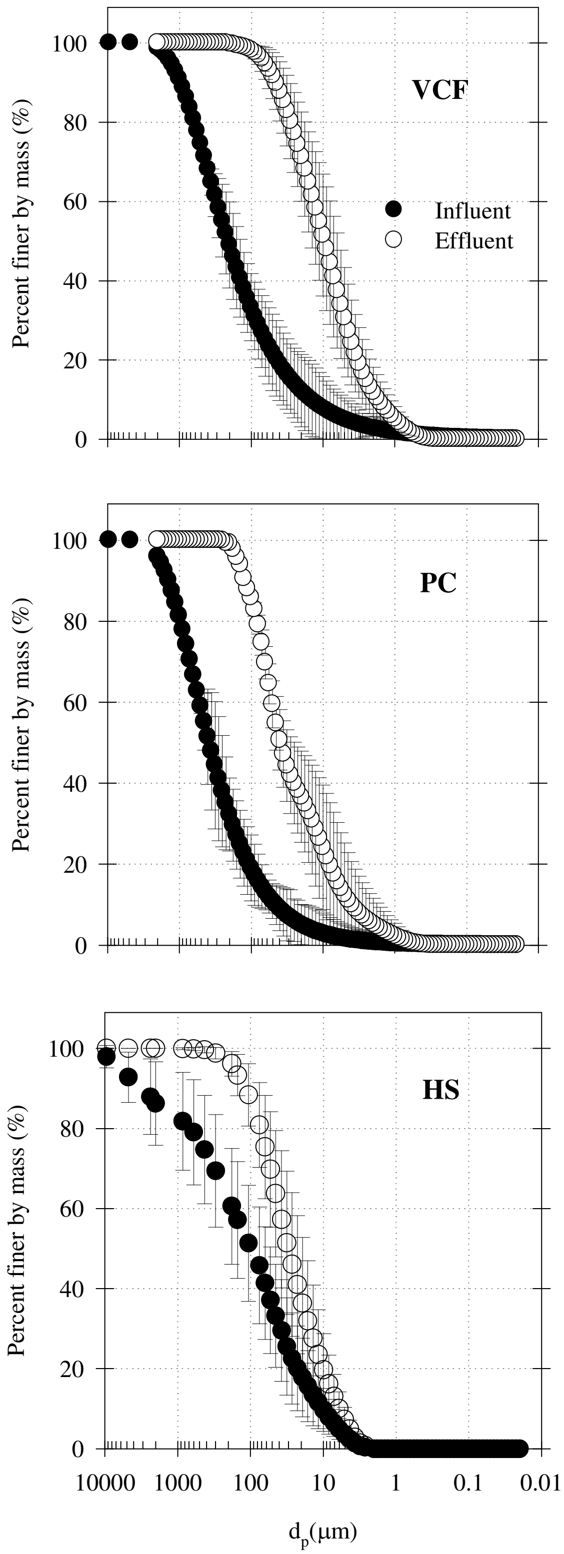
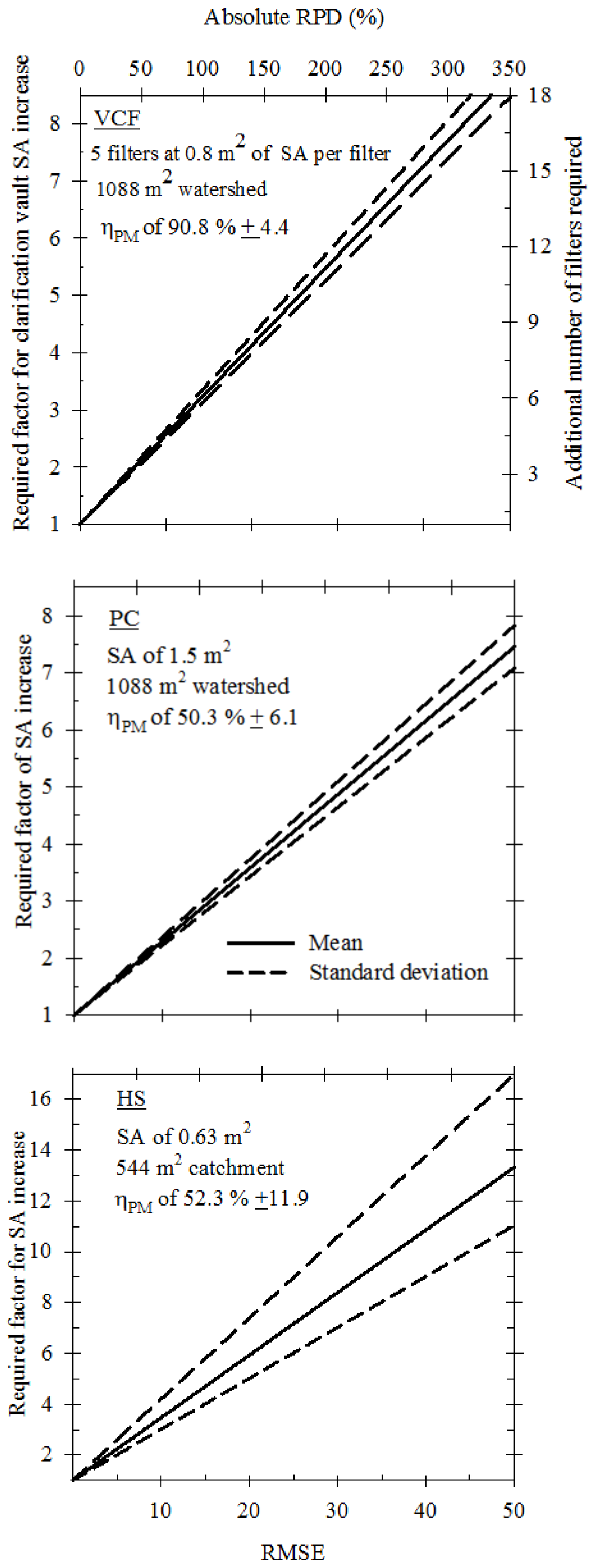

VCF: Sedimentation & Filtration
$f_n = 0.4\, e^{-6.2\, Q}$
$Q_{max} = 25$ L/s
$Q_{50} = 0.1$ L/s
n = 3926
HS: Hydrodynamic Separation
$f_n = 0.6\, e^{-7.1\, Q}$
$Q_{max} = 17.5$ L/s
$Q_{50} = 0.5$ L/s
n = 3098
PC: Sedimentation
$f_n = 0.6\, e^{-5.4\, Q}$
$Q_{max} = 26$ L/s
$Q_{50} = 1.9$ L/s
n = 1866
Normalized Frequency, f_n
Normalized Q (L/s)
0.0
0.2
0.4
0.6
0.8
1.0

Figure S1.



VCF
Influent
Effluent
PC
HS
Percent finer by mass (%)
100
80
60
40
20
0
10000
1000
100
10
1
0.1
0.01
d_p(μm)

Figure S2.



Absolute RPD (%)
0
50
100
150
200
250
300
350
Required factor for clarification vault SA increase
Additional number of filters required
VCF
5 filters at 0.8 m2 of SA per filter
1088 m2 watershed
ηPM of 90.8 % ± 4.4
PC
SA of 1.5 m2
1088 m2 watershed
ηPM of 50.3 % ± 6.1
Required factor of SA increase
Mean
Standard deviation
HS
SA of 0.63 m2
544 m2 catchment
ηPM of 52.3 % ±11.9
Required factor for SA increase
10
20
30
40
50
RMSE

Figure S3.

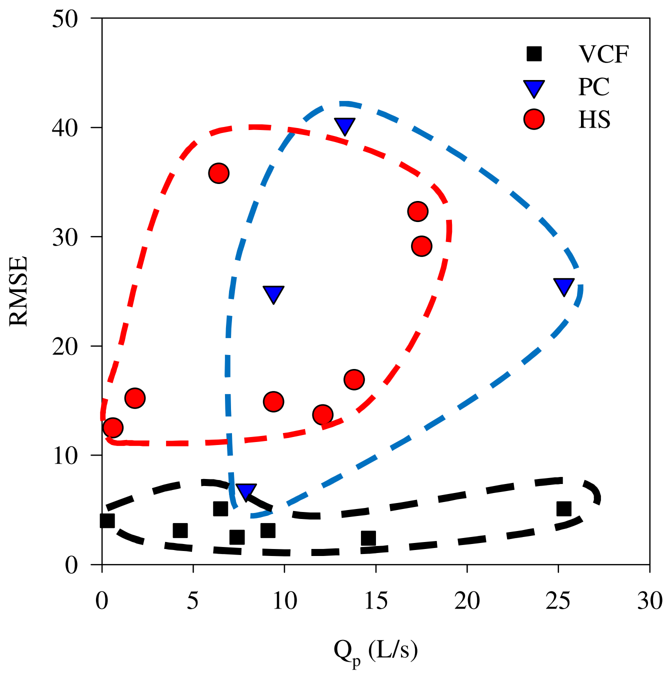
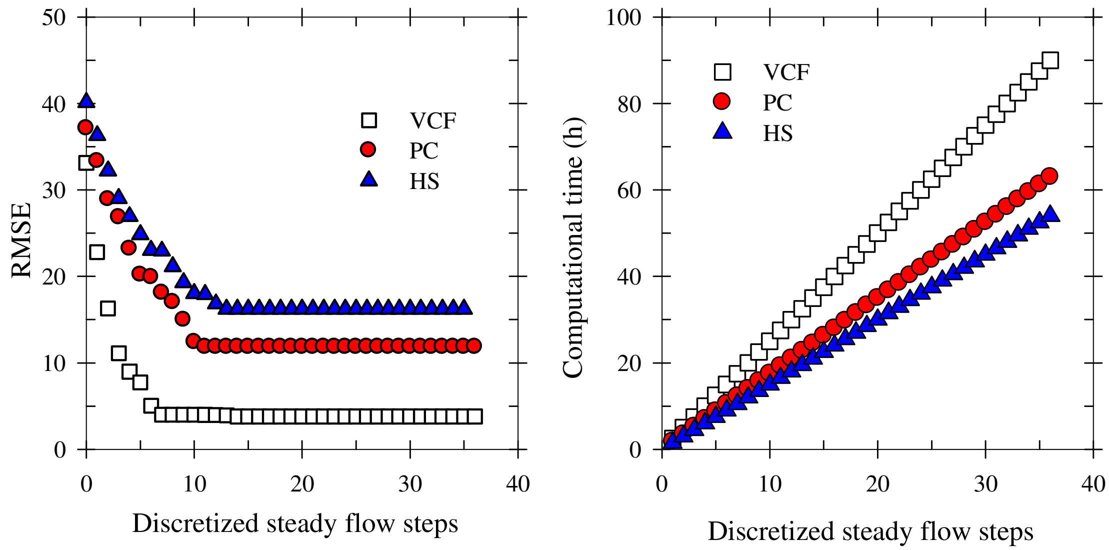


Figure S4.



RMSE
VCF
PC
HS
Discretized steady flow steps
Computational time (h)
VCF
PC
HS
Discretized steady flow steps

Figure S5.