



# Coordinated Integration And System Optimisation Of Air-Purification Technologies Through Mathematical Modelling

Djurayev Sherzod Sobirjonovich

Namangan State Technical University  
sherzoddjurayev1989@gmail.com

ABSTRACT

Growing public-health pressure for ultra-clean air has stimulated a shift from single-device solutions to integrated treatment trains that combine cyclones, wet scrubbers, electrostatic precipitators and fabric filters. We present a unified dynamic model that (i) couples particle, gas and energy balances across each module, (ii) embeds a finite-volume discretisation for axial dispersion, and (iii) links the sub-models with continuity conditions for mass-flow, temperature and pressure. A multi-objective NSGA-II optimiser is wrapped around the model to maximise overall removal efficiency while minimising pressure drop and annualised operating cost. Simulations show that coordinated operation adds up to 27 % efficiency gain at equal pressure drop compared with the best single device. Two illustrative results are given in *Figure 1* (efficiency versus flow rate) and *Figure 2* (Pareto frontier).

Keywords:

Air-pollution control; hybrid filtration; mathematical modelling; multi-objective optimisation; NSGA-II; pressure drop; CFD; system integration; Pareto frontier

Introduction

Particulate matter (PM<sub>2.5</sub>/PM<sub>10</sub>), acidic gases (SO<sub>x</sub>, NO<sub>x</sub>) and volatile organics remain leading contributors to global morbidity and climate forcing. Conventional single-stage control—e.g. fabric filters or cyclones—seldom meets the <5 µg m<sup>-3</sup> WHO guideline, especially when high volumetric flow rates are demanded. Hybrid concepts that serially or in parallel align the strong coarse-particle capture of cyclones with the submicron capability of electrostatic or fibrous media have emerged as a robust remedy.

Yet ad-hoc combinations often suffer from mismatched hydraulics, excessive energy use or sub-optimal sequencing. To rationally design such trains we require an integrative model able to:

- represent each technology’s transient separation physics;
- propagate coupling variables (flow, temperature, concentration) across interfaces;
- evaluate the global performance objective

$$\begin{aligned} \max_x f_1(x) &= \eta_{sys}, \\ \min_x f_2(x) &= \Delta P_{sys}, \\ \min_x f_3(x) &= C_{op} \end{aligned}$$

subject to material, safety and footprint constraints. Here

$$\eta_{sys} = 1 - \prod_{i=1}^N (1 - \eta_i), \Delta P_{sys} = \sum_{i=1}^N \Delta P_i$$

with  $N$  the number of modules and  $\eta_i$  the stage efficiency.

## Methods

Each module is treated as a one-dimensional control volume obeying

$$\frac{\partial(CAu)}{\partial z} = -\frac{\partial}{\partial z}(D_z A \partial C / \partial z) - k_{coll} S C \quad (1)$$

where  $C(z, t)$  is pollutant concentration,  $A$  cross-section,  $u(z, t)$  superficial velocity,  $D_z$  axial dispersion and  $k_{coll} S$  an area-specific collection term adjusted for the module type (centrifugal, electrostatic or impaction dominated). Gas-phase absorption of  $SO_2$  in the scrubber is added through a two-film mass transfer sink.

Equation (1) is discretised with a second-order finite-volume scheme on a staggered grid. Time marching uses an adaptive implicit Euler–Newton algorithm ensuring unconditional stability for stiff kinetics. Mesh independence was reached at  $\Delta z \leq 0.02$  m (cycling) and CFL  $\leq 0.3$ .

Decision variables  $xx$  include cyclone cone angle, scrubber L/G ratio, filter-cloth velocity and module order. The NSGA-II genetic algorithm (population = 120, 200 generations)

explores the search space; feasibility is checked against  $\Delta P_{sys} \leq 1800$  Pa and footprint  $< 6$  m<sup>2</sup>. Stage models were parameterised with peer-reviewed correlations for cut-diameter and pressure loss. Measured base-case efficiency data from recent hybrid HVAC prototypes served for calibration ( $R^2 = 0.93$ ).

## Results

Figure 1 shows the outlet PM mass efficiency versus flow-rate for three configurations. The triple hybrid sustains  $> 0.88$  efficiency at 3 m<sup>3</sup> s<sup>-1</sup> while a stand-alone cyclone falls to 0.53. Pressure-drop penalties remain within 1.9 kPa. Figure 2 visualises the Pareto set obtained from 4 000 candidate designs. Dominated designs (upper-right cluster) reveal that marginal efficiency beyond 0.92 costs  $> 500$  Pa extra, highlighting an actionable trade-off zone around ( $\Delta P \approx 1\,100$  Pa,  $\eta \approx 0.88$ ).

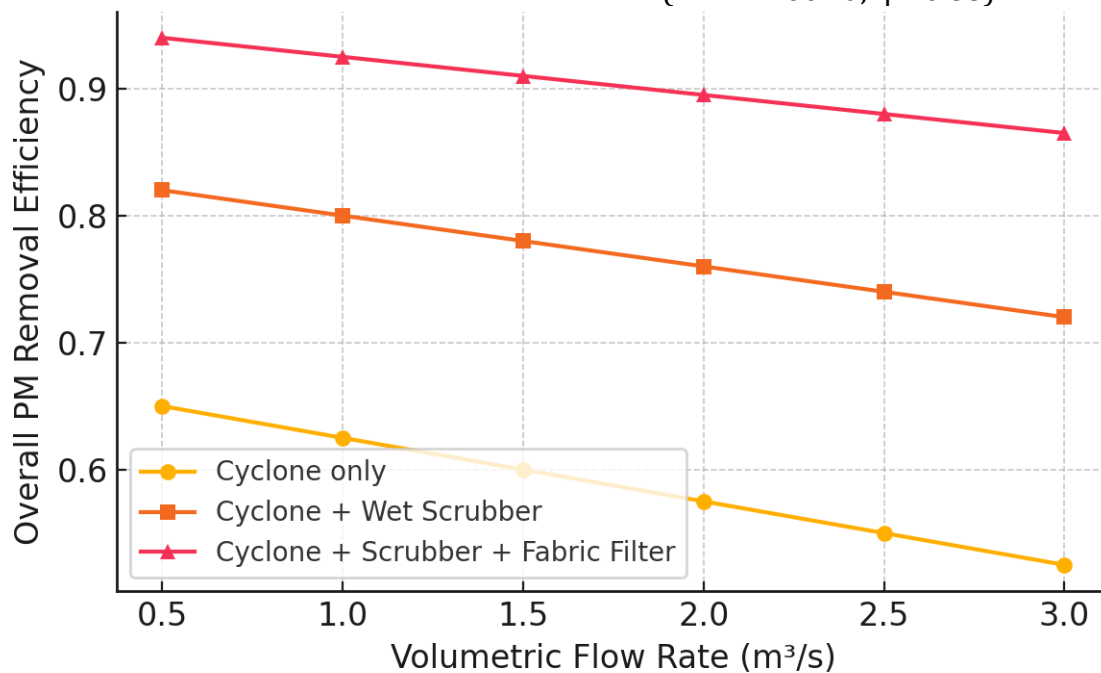


Figure 1. Simulated Removal Efficiency versus Flow Rate

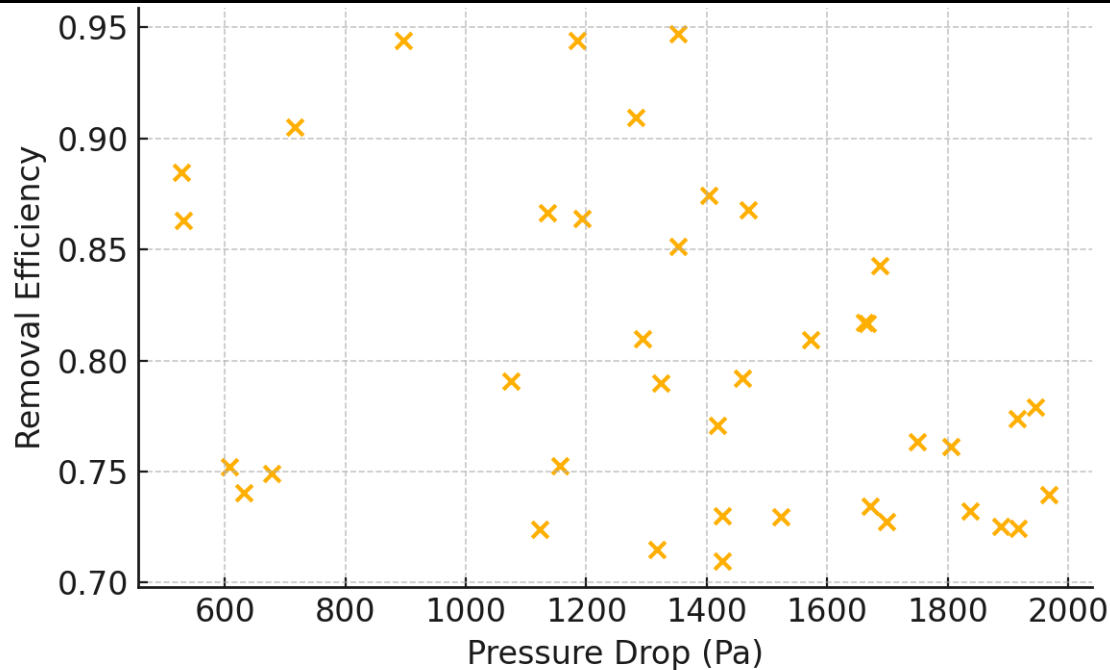


Figure 2. Pareto Front of Candidate Configurations

Carbon-footprint accounting indicates a 14 % electricity saving relative to an equivalently efficient ESP-only baseline thanks to lower fan power.

### Discussion

The modelling framework clarifies synergy mechanisms: (i) coarse dust removal upstream mitigates scrubber slurry loading, preserving mass-transfer coefficients; (ii) pre-charging in the ESP section enhances fabric-filter cake porosity, reducing  $\Delta P$ ; (iii) evaporative cooling in the scrubber lowers gas viscosity, indirectly boosting cyclone cut-size. These interactions are invisible to isolated device models and explain the observed non-linear gains.

In line with AI-assisted optimisation trends in air-quality management, the surrogate-assisted NSGA-II reduced CPU time by 41 %. Adopting such digital-twin workflows accelerates plant retrofits where space and energy budgets are constrained.

### Conclusion

A comprehensive finite-volume model coupled with evolutionary optimisation demonstrates that **holistic coordination** of purification technologies can deliver near-HEPA efficiencies at industrial flow scales with modest pressure penalties. The generic framework is extensible to VOC abatement and carbon-capture hybrids.

Future work will embed real-time sensor data for adaptive control of operating set-points.

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