Table S2. Regression coefficients (*a, b*) with standard errors (in parentheses), in the best-fit function of $F_{48} = a \cdot RH + b$ for chloroacetanilide and dinitroaniline herbicides

	Chloroacetanilides				Dinitroanilines		
	alachlor	butachlor	metolachlor	propachlor	pendimethalin	prodiamine	trifluralin
$PM_{2.5}$-loaded QFF							
a	0.40 (0.14)	0.04 (0.02)	0.07 (0.04)	1.22 (0.20)	0.93 (0.11)	0.60 (0.08)	0.51 (0.16)
b	0.04 (0.06)	0.03 (0.01)	0.02 (0.02)	0.09 (0.08)	0.18 (0.05)	0.07 (0.04)	0.65 (0.07)
R^2	0.73	0.69	0.46	0.93	0.96	0.94	0.77
bare QFF							
a	0.22 (0.05)	0.00 (0.01)	0.03 (0.01)	0.78 (0.04)	0.98 (0.10)	0.63 (0.09)	0.40 (0.06)
b	-0.01 (0.02)	0.03 (0.01)	0.02 (0.00)	0.08 (0.02)	0.09 (0.04)	-0.01 (0.04)	0.72 (0.03)
R^2	0.91	0.04	0.85	1.00	0.98	0.96	0.96

Table S3. Estimation of $P_{L,}{}^{o}{}_{8°C}$ for study herbicides

Herbicide family	Common name	Estimated $P^{0}_{L,8^{\circ}C}$ (Pa)
Chloroacetanilide	alachlor	8.24×10^{-4}
	butachlor	7.72×10^{-5}
	metolachlor	8.36×10^{-4}
	propachlor	2.00×10^{-2}
Dinitroaniline	pendimethalin	1.61×10^{-3}
	prodiamine	6.29×10^{-6}
	trifluralin	2.10×10^{-3}

The $P^{o}_{L,8^{\circ}C}$ values were corrected from literature $P^{o}_{L,25^{\circ}C}$ values using the Clausius-Clapeyron Equation (6). The experimental enthalpies of volatilization for alachlor and metolachlor were determined to be 69.6 and 64 kJ/mol, respectively (7) and ACD/Solaris model values for these two herbicides were 65.86 and 65.54 kJ/mol, respectively (7). Values for the enthalpy of volatilization are not available for the other five herbicides; therefore, based on the experimental

and model values of alachlor and metolachlor, a mean value of 66 kJ/mol was estimated as the enthalpy of volatilization for calculating $P^{o}_{L,8^{\circ}C}$.

Table S4. Estimated $K_{OA,8°C}$ values for study herbicides.

Herbicide family	Common name	Estimated $K_{OA,8°C}$ (mol/Pa·m^3)
Chloroacetanilide	alachlor	3.93×10^{6}
	butachlor	6.12×10^{6}
	metolachlor	1.48×10^{6}
	propachlor	1.63×10^{4}
Dinitroaniline	pendimethalin	1.75×10^{6}
	prodiamine	1.41×10^{5}
	trifluralin	2.09×10^{4}

The $K_{OA,8°C}$ was estimated for each herbicide as the ratio $K_{OW,8°C}/K_{H,8°C}$ because no experimental data are available in the literature (8). The temperature dependence on K_{OW} was assumed to be negligible, so $K_{OW,8°C}$ was assumed to be equal to $K_{OW,25°C}$. The $K_{H,8°C}$ for study herbicides are in Table S5.

Table S5. $K_{H,\ 8°C}$ for study herbicides

Herbicide family	Common name	Estimated $K_{H,8°C}$ (Pa·m^3/mol)
Chloroacetanilide	alachlor[a]	7.65×10^{-4}
	butachlor[b]	4.40×10^{-4}
	metolachlor[a]	5.81×10^{-4}
	propachlor[b]	1.79×10^{-3}
Dinitroaniline	pendimethalin[b]	3.26×10^{-2}
	prodiamine[b]	1.95×10^{-2}
	trifluralin[a]	5.45

The dependency of K_H on temperature has been experimentally determined for metolachlor, alachlor and trifluralin (*5, 9, 10*). For propachlor, butachlor, pendimethalin and prodiamine, the 2D increment model was used to approximate the air/water phase transition enthalpy (ΔH^{ϕ}) from the herbicide structure (*11*), and the $K_{H,8°C}$ was then calculated. [a] $K_{H,8°C}$ extrapolated from literature data; [b] $K_{H,8°C}$ estimated using 2D increment model (11).

Table S6. Estimated solvation properties for study herbicides

	$\sum \alpha_2^H$ H-donor	$\sum \beta_2^H$ H-acceptor	$\log K_{hexadecane/air}$ (25 °C)	π_2^H (S)	R_2 (E)	V	# H-bond donors	# H-bond acceptors	TPSA
Alachlor	0.0	0.94	9.362	1.63	1.11	2.1402	0	3	29.54
Butachlor	0.0	0.95	10.845	1.64	1.11	2.5629	0	3	29.54
Metolachlor	0	0.98	9.742	1.62	1.12	2.2811	0	3	29.54
Propachlor	0.0	0.76	7.436	1.57	1.04	1.6588	0	2	20.31
Pendimethalin	0.05	0.57	10.235	1.59	1.42	2.1509	1	7	109.69
Prodiamine	0.23	0.77	10.460	2.01	1.30	2.3035	2	8	126.92
Trifluralin	0.00	0.55	9.390	1.84	0.99	2.2037	0	7	100.9

π_2^H = Abraham's polarity/polarizability parameter; R_2 = Excessive molar refraction; V = McGowan's characteristic volume (cm^3 $mol^{-1}/100$); TPSA = topological polar surface area ($Å^2$). Estimated from Abraham type equations using the ADME Boxes software (Ver 3.0; http://www.ap-algorithms.com/absolv.htm).

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