Performance Comparison of Agilent 1290 Infinity Binary and Quaternary Systems as an MS Front-End

Technical Overview

Authors

Edgar Naegele,
Angelika Gratzfeld-Huesgen
Agilent Technologies, Inc.
Waldbronn, Germany

Abstract

This Technical Overview demonstrates the performance of the Agilent 1290 Infinity Binary as well as the Agilent 1290 Infinity Quaternary LC System as a front-end for mass spectrometry. Performance data about calibration linearity, sensitivity, and precision is shown for a suite of pesticide compounds.

Verified for Agilent
1290 Infinity II LC

Agilent Technologies

Introduction

Binary pumps with high-pressure mixing as well as quaternary pumps with low-pressure mixing can be used as front-end LC systems for LC/MS systems. Typically, depending on their different delay volumes, the gradient reaches the column at different times for the same applied gradient resulting in different retention times of the compounds.

Conversely, different types of pumps create gradients differently by putting packages of the solvents together and mixing them before the final composition leaves the pump. Therefore, it is not evident that the performance for calibration linearity, sensitivity, and precision is in the same range for different types of pumps. To confirm that both types of pumps can be used as front-end for LC/MS, the same performance data concerning calibration linearity, sensitivity, and precision was acquired and compared. A suite of pesticide compounds was chosen to be used as an example.

Experimental

Equipment

- Agilent 1290 Infinity Binary Pump (G4220A)
- Agilent 1290 Infinity Quaternary Pump (G4220A)
- Agilent 1290 Infinity Autosamlper (G4226) with Thermostat (G4220A)
- Agilent 1290 Infinity Thermostatted Column Compartment (G1316C)
- Agilent G6490 Triple Quadrupole LC/MS with Agilent Jet Stream Technology

Column

Agilent ZORBAX RRHD Eclipse Plus C18, 2.1 × 50 mm, 1.8 µm (p/n 959757-902)

Software

- Agilent MassHunter Data Acquisition Software for triple quadruple mass spectrometer, Version 06.00
- Agilent MassHunter Optimizer Software, Version 06.00
- Agilent MassHunter Qualitative Software, Version 06.00
- Agilent MassHunter Quantitative Software, Version 06.00

Chemicals and standards

All solvents were LC/MS grade. Acetonitrile was purchased from J.T. Baker, Germany. Fresh ultrapure water was obtained from a Milli-Q Integral system equipped with LC-Pak Polisher and a 0.22-µm membrane point-of-use cartridge (Millipak).

A standard mixture containing 10 ng/µL each of 17 pesticides in acetonitrile solution was obtained from Dr. Ehrenstorfer GmbH (Pesticide Mix 44, part no. 18000044 - Dr. Ehrenstorfer GmbH Bgm.-Schlosser-Str. 6 A, 86199 Augsburg, Germany).

LC Method	
Solvents	A) Water + 5 mM ammonium formate B) Acetonitrile
Flow rate	0.5 mL/min
Gradient	0 minutes – 20 % B, 5 minutes – 40 % B, 6 minutes – 40 % B, 7 minutes – 75 % B, 8 minutes – 95 % B Stop time 10 minutes Post time 3 minutes
Injection volume	2 µL
Injection with needle wash	10 seconds methanol in flush port
Sample temperature	8 °C
Column temperature	40 °C
MS Method	
Capillary	3,500 V
Nozzle voltage	300 V
Sheath gas flow	12 L/min
Sheath gas temperature	375 °C
Nebulizer	30 psi
Gas flow	15 L/min
Gas temperature	125 °C
Polarity	Positive
MRM method	Product ions for quantifier and qualifier and their collision energies for the fragmentation were determined and optimized with the MassHunter Optimizer software (details not shown here)

Results and Discussion

For the creation of the calibration curves and the determination of the limit-of-quantification (LOQ) as well as the limit-of-detection (LOD), the pesticide standard solution was diluted to 200 ppt. This stock solution was further diluted with a 1:5 dilution pattern down to 0.0128 ppt. The measurement of the 40 ppt dilution with both LC front-end configurations (binary as well as quaternary pump) showed a shift in the retention time according to the difference in delay volume of the pumps. The quaternary pump showed the higher values for the retention time of the individual compounds (Figure 1). For instance, metolachlor, the last eluting compounds shows a delay time of approximately 0.75 minutes. At the given flow rate, this is equal to the delay volume of approximately 375 µL. The complete dilution series was measured to create calibration curves as well as to find LODs and LOQs. The linearity coefficients determined from the measurement with both pump configurations of all compounds are better than 0.99990. Table 2A summarizes the measured values for the binary pump configuration.

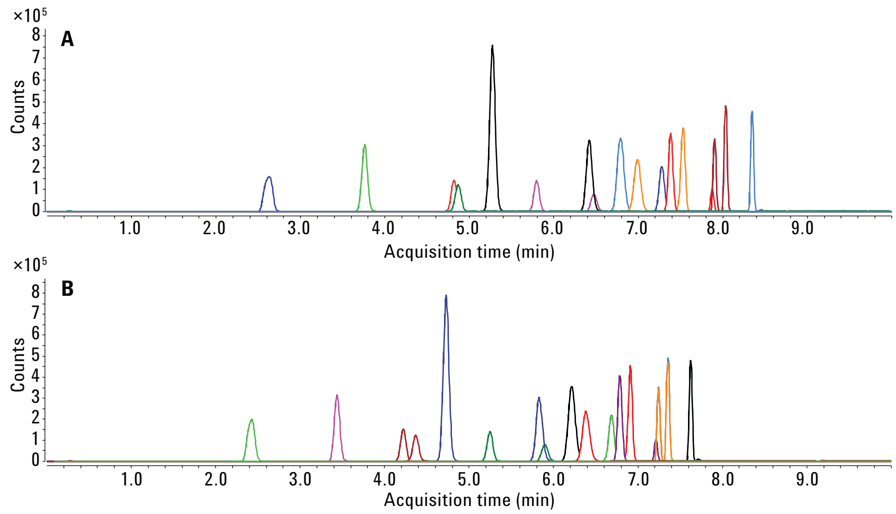

Figure 1. Separation of a mixture of 17 pesticides by a gradient driven with A) quaternary pump and B) binary pump. Due to the higher delay volume of the quaternary pump, these retention time have the higher values.

Table 2A. Performance of the MS front end LC comprising the binary pump.

	R.T. (min)	R.T. RSD (%)	Area RSD (%)	Linearity	LOQ (ppt)	LOD (ppt)
Atrazine desethyl	2.47	0.37	1.13	0.99991	35.0	9.0
Metoxuron	3.43	0.29	2.11	0.99995	47.0	7.6
Cyanazine	4.34	0.41	2.01	0.99994	22.0	12.0
Simazine	4.38	0.27	1.68	0.99996	29.0	9.0
Hexazinone	4.72	0.26	1.53	0.99992	9.3	2.5
Monolinuron	5.25	0.29	1.03	0.99995	45.0	13.0
Chlorotoluron	5.83	0.28	1.87	0.99994	18.0	4.8
Metobromuron	5.89	0.29	1.13	0.99997	70.0	22.0
Methabenzthiazuron	6.22	0.21	2.15	0.99994	16.0	7.6
Atrazine	6.39	0.15	1.67	0.99994	30.0	9.0
Diuron	6.68	0.11	2.28	0.99992	39.0	11.0
Isoproturon	6.78	0.08	1.69	0.99994	14.5	4.4
Metazachlor	6.91	0.03	2.38	0.99995	15.0	4.8
Linuron	7.21	0.03	1.91	0.99992	85.0	23.0
Sebuthylazine	7.24	0.03	1.52	0.99997	26.5	7.8
Terbuthylazine	7.35	0.02	2.16	0.99992	21.5	6.5
Metolachlor	7.62	0.02	2.94	0.99993	6.5	2.5

Table 2B summarizes the values measured for the quaternary pump configuration, and Figure 2 shows the range of linearity coefficients for selected compounds. The LOQs with a signal-to-noise ratio (S/N) of 10 are on average 30 ppt for both LC configurations and the LODs with an S/N of 3 are below 10 ppt for most compounds for both LC configurations.

Table 2B. Performance of the MS front end LC comprising the quaternary pump.

	R.T. (min)	R.T. RSD (%)	Area RSD (%)	Linearity	LOQ (ppt)	LOD (ppt)
Atrazine desethyl	2.67	0.65	0.91	0.99994	30.0	6.0
Metoxuron	3.80	0.43	1.52	0.99993	38.0	6.0
Cyanazine	4.83	0.26	2.77	0.99990	28.0	8.0
Simazine	4.93	0.22	2.78	0.99998	32.0	9.0
Hexazinone	5.32	0.18	1.03	0.99995	29.0	6.0
Monolinuron	5.86	0.22	2.11	0.99996	60.0	15.0
Chlorotoluron	6.47	0.22	1.98	0.99993	21.0	5.0
Metobromuron	6.53	0.19	1.66	0.99996	64.0	20.0
Methabenzthiazuron	6.74	0.26	2.03	0.99996	7.2	2.2
Atrazine	7.04	0.17	2.04	0.99993	25.0	7.5
Diuron	7.33	0.23	1.73	0.99991	42.0	8.0
Isoproturon	7.43	0.14	1.47	0.99998	12.0	3.6
Metazachlor	7.56	0.08	2.37	0.99998	12.0	3.6
Linuron	7.89	0.06	1.18	0.99998	80.0	25.0
Sebuthylazine	7.92	0.04	2.46	0.99991	32.0	9.6
Terbuthylazine	8.04	0.04	2.38	0.99996	22.0	6.7
Metolachlor	8.37	0.04	3.03	0.99996	5.3	1.6

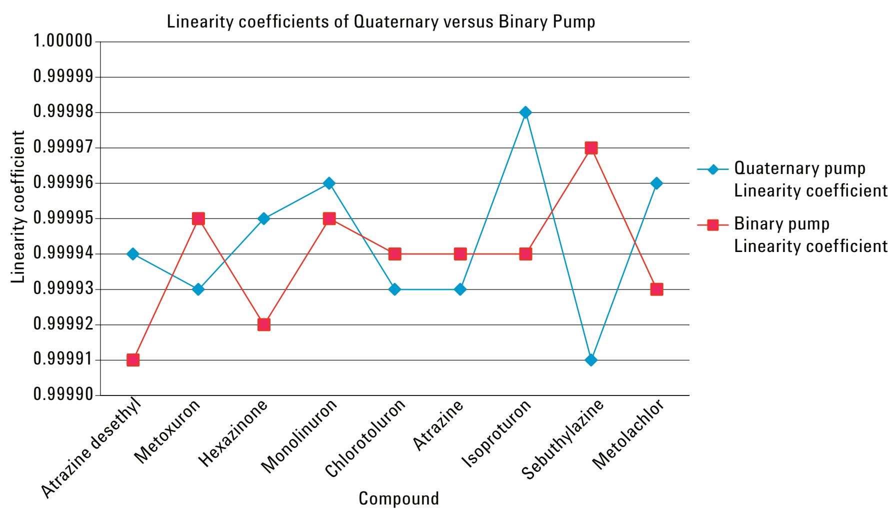

Figure 2. Linearity coefficients of selected pesticide compounds eluting over the complete retention time range showing linearity for binary as well as quaternary pump configuration.

Selected compounds covering the complete elution range show that LOQs as well as LODs were in the same concentration range for both configurations with the typical trend, that later eluting compounds show higher sensitivity due to better focusing effects on the column and improved ionization efficiency due to the higher organic solvent ratio (Figure 3).

For a statistical evaluation of retention time and precision, the 40 ppt sample was used and injected 12 times. For both configurations, the retention time RSD was typically below 0.3 %, and the area RSD was typically below 2.5 % (Figures 4 and 5).

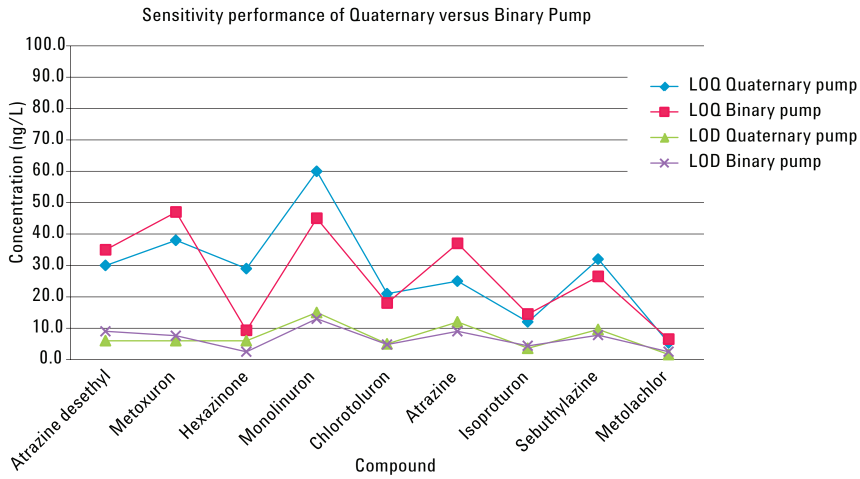

Figure 3. Sensitivity performance of selected pesticide compounds eluting over the complete retention time range showing LOQs and LODs for binary as well as quaternary pump configuration.

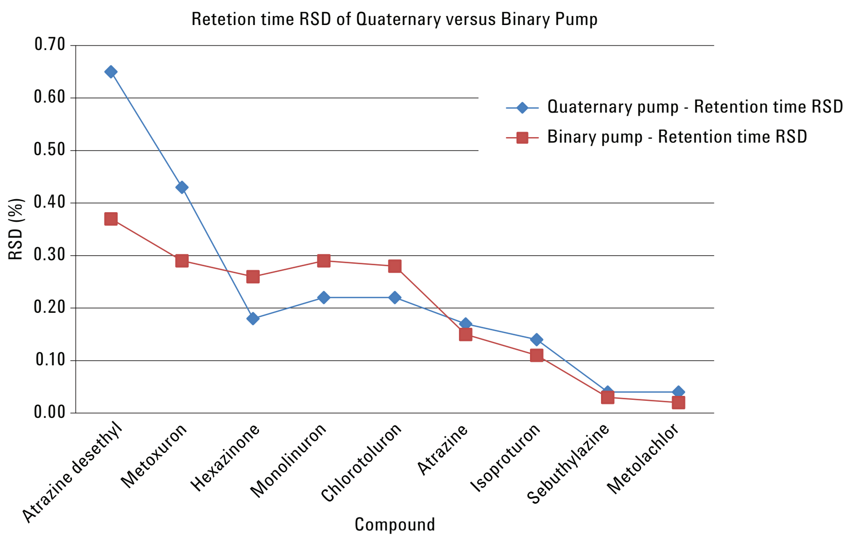

Figure 4. Retention time precision (RSD) of selected pesticide compounds eluting over the complete retention time range for binary as well as quaternary pump configuration.

Conclusion

This Technical Overview demonstrates that front-end LC systems for mass spectrometry including the Agilent 1290 Infinity Binary Pump or the Agilent 1290 Infinity Quaternary Pump give the same performance concerning sensitivity (LOQ and LOD), linearity, retention time, and area precision. The only difference was that the quaternary pump gradient resulted in higher retention times due to the higher delay volume.

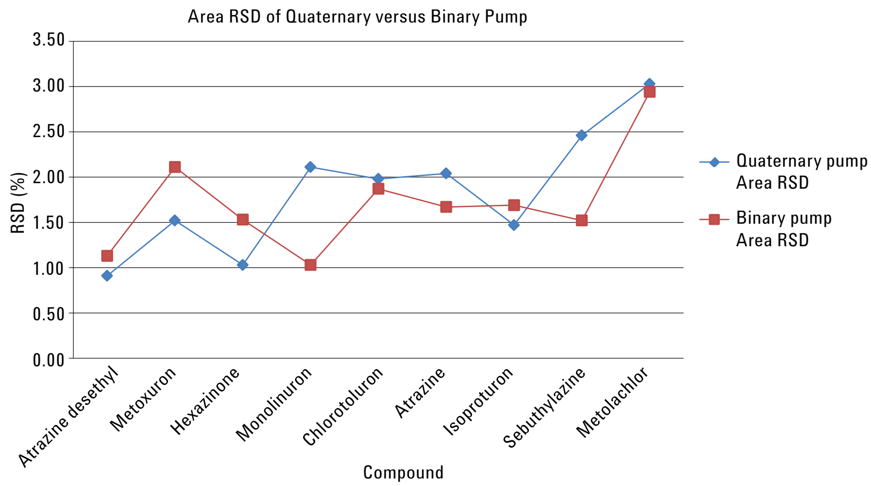

Figure 5. Area precision (RSD) of selected pesticide compounds eluting over the complete retention time range for binary as well as quaternary pump configuration.

www.agilent.com/chem

Published in the USA, September 15, 2014
5991-3211EN

Agilent Technologies