Application Note

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Analysis of Trace Impurities in Monocyclic Aromatic Solvents Following ASTM D7504

Dual simultaneous analysis using the Agilent 8860B gas chromatograph

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Abstract

This study presents the dual-channel Agilent 8860B gas chromatograph (GC) system for analyzing the impurities of monocyclic aromatic solvents in accordance with American Society for Testing and Materials (ASTM) D7504. Methodological validation confirmed that column resolution, sensitivity, and quantitation accuracy meet standard requirements. Mass concentration precision (RSDs) achieved is below 1% for most of the impurities. Both channels produced consistent results within the reproducibility limits of ASTM D7504. This application note demonstrates three methods that meet ASTM D7504 requirements using helium, nitrogen, and hydrogen carrier gas. Meanwhile, the normalization quantification based on compound's effective carbon number can be easily realized using Agilent OpenLab CDS software. The 8860B GC together with the OpenLab CDS system provides a complete and verified solution for aromatic impurity analysis, covering the whole workflow from sample preparation, separation, and detection to final report generation.

Introduction

The production of high-purity monocyclic aromatic hydrocarbons, such as benzene, toluene, ethylbenzene, and xylenes (BTEX), is a cornerstone of the modern petrochemical industry. These compounds serve as essential feedstocks for the synthesis of plastics, resins, and textiles. Because even trace impurities can adversely affect downstream chemical reactions and product quality, rigorous analytical testing is required to ensure these intermediates meet strict commercial specifications.

ASTM D7504 is the industry-standard test method for determining the purity of, and trace impurities in, monocyclic aromatic hydrocarbons using gas chromatography (GC) with flame ionization detector (FID).[1] This method is favored for its streamlined workflow; it utilizes effective carbon number (ECN) correction factors for area normalization. This eliminates the need for labor-intensive, multipoint calibrations for every individual impurity, allowing laboratories to calculate purity and quantify trace nonaromatics and aromatics with high precision.

The application scope of ASTM D7504 covers a wide array of aromatic liquids, including benzene, toluene, mixed xylenes, and styrene. To comply with the method's stringent performance requirements, the GC system must demonstrate:

- **High sensitivity:** A limit of quantitation (LOQ) of at least 0.0006% by mass.
- **Good resolution:** Maintaining a valley-to-peak ratio of no more than 50% for critical separations (such as *p*-xylene and *m*-xylene).
- **Strict precision:** Highly reproducible peak areas to ensure accurate purity calculations.

Implementing ASTM D7504 on a dual-channel GC/FID platform—where two independent analytical channels configured with identical injectors, columns, and detectors operate within a single GC oven—provides significant operational advantages:

1. **Enhanced laboratory throughput:** By performing two injections simultaneously, the test lab can double its sample capacity per instrument, effectively reducing the cost-per-analysis and maximizing hardware ROI.
2. **Method flexibility and redundancy:** A dual-channel set up allows a lab to run different sample types (such as toluene on the front channel and xylene on the back) in a single oven cycle. Furthermore, it provides an immediate "back up" channel to maintain uptime during routine maintenance.

For the system to be considered reliable, both channels should meet ASTM D7504 sensitivity, resolution, and precision requirements. In addition, both channels should yield consistent quantitative results for the same sample. The reproducibility limit (R) demonstrated in ASTM D7504 interlaboratory testing will be used to evaluate the result consistency between the two channels.

ASTM D7504 recommends helium and hydrogen as carrier gas. In China, major Chinese petrochemical companies often align their internal quality control standards directly with ASTM D7504 when testing for export of high-purity chemical intermediates. Because nitrogen is commonly used in China, they commonly adapt the ASTM D7504 method to use nitrogen carrier gas.

This application note demonstrates how dual-channel analysis on the Agilent 8860B GC, following ASTM D7504, delivers consistent and high-precision data using three types of carrier gas.

Experimental

An Agilent 8860B GC was configured with dual split/splitless inlets and dual flame ionization detectors (FIDs). The sample introduction was made by dual Agilent 7693A automatic liquid samplers (ALS) with high density turrets (16-vial). The analytical parameters and consumables are summarized in Tables 1 and 2. Data acquisition and analysis were conducted using Agilent OpenLab CDS version 2.8.

Table 1. The system analytical parameters using three carrier gas.

ALS and Inlets			
Injection Volume	0.6 µL		
Mode	Split, 100:1		
Temperature	260 °C		
Carrier Gas	He, 2.1 mL/min	H_2, 1.7 mL/min	N_2, 1.2 mL/min
Oven Temperature			
	He Method	**H_2 Method**	**N_2 Method**
Initial Temperature	60 °C	60 °C	60 °C
Initial Hold	10 min	10 min	15 min
Ramp 1 Rate	5 °C/min	5 °C/min	3.5 °C/min
Ramp 1 Set Point	150 °C	150 °C	150 °C
Ramp 1 Hold	0 min	0 min	0 min
Ramp 2 Rate	30 °C/min	30 °C/min	30 °C/min
Ramp 2 Set Point	220 °C	220 °C	220 °C
Ramp 2 Hold	8 min	8 min	8 min
Post Run Temperature	0 °C	0 °C	0 °C
Post Run Time	0 min	0 min	0 min
Detector			
Temperature	260 °C		
Air	400 mL/min		
Hydrogen	30 mL/min		
Make-Up (N_2)	25 mL/min		

Table 2. Column and consumables.

Configuration	
Column	Agilent J&W HP-INNOWax, 60 m × 0.32 mm, 0.5 µm (p/n 19091N-216I)
Consumables	
Inlet Septa	Agilent nonstick advanced green (p/n 5183-4759)
Inlet liner*	Agilent ultra inert, low pressure drop split liner with glass wool (p/n 5190-2295)
ALS Syringes	Agilent Blue Line autosampler syringe, 5 µL, fixed needle, 23-26s/42/cone (p/n G4513-80206)
Column Ferrules	Short graphite for 0.32 mm columns, 10/pack (p/n 5080-8853)

* The deactivated split liner (p/n 5183-4647) is verified and also can be used for this application.

Chemicals and reagents

Twenty-three chemicals were purchased from ANPEL Laboratory Technologies (Shanghai) Inc. They are common impurities found in the monocyclic aromatic solvents and dissolved in *n*-hexane to ~ 0.1% mass concentration for identification of each impurity. The impurity mixture was used for analytical method optimization. For column resolution and method recovery evaluation, *p*-xylene check standard number one is purchased from AccuStandard Inc.

Lab made check standards containing common contaminants for benzene, toluene, and *p*-xylene were prepared according to the sample composition in previous work for precision test.[2] Benzene in *p*-xylene (0.0006% wt) was prepared to evaluate system sensitivity. Detailed sample compositions are shown in Table 3.

Table 3. Compositions of test standards.

Compound	Benzene Check Standard (Mass %)	Toluene Check Standard (Mass %)	*p*-Xylene Check Standard (Mass %)	*p*-Xylene Standard No. 1 (Mass %)	LOD Test Standard (Mass %)
n-C_6	0.032	–	0.003	–	
n-C_9	–	–	–	0.017	
Benzene	99.91	0.016	0.003	0.02	0.0006
Toluene	0.009	99.92	0.034	0.02	
1,4-Dioxane	0.002	–	–	–	
Ethylbenzene	–	0.027	0.245	0.1	
p-Xylene	0.005	0.013	99.23	99.62	
m-Xylene	0.005	0.016	0.376	0.101	
Cumene	0.002	–	–	0.02	
o-Xylene	0.004	0.0020	0.09	0.102	
Propylbenzene	0.018	0.0030	–	–	
Butylbenzene	0.009	–	0.009	–	
p-Diethylbenzene	–	–	–	0.02	

Results and discussion

Method development for helium, nitrogen, and hydrogen carrier gas

The helium- and hydrogen-based methods utilized the oven temperature program recommended by ASTM D7504. The helium column flow rate used in previous work was reused.[3] The hydrogen column flow rate was optimized with 19 of the 23 typical impurities in monocyclic aromatic solvents separated at baseline level.

The nitrogen method oven temperature program was developed based on the helium method using method translator. The average linear velocity of the helium method is 29 cm/sec. Theoretically, the optimum linear velocity for nitrogen is between 10 to 15 cm/sec. To balance the analytical speed and resolution, the nitrogen average linear velocity started from 20 cm/sec, with the oven ramp rate around 70% of the helium method as shown in Figure 1.

To apply the nitrogen method to the 23-impurity mixture for separation check, minor adjustments were made on the initial temperature program, extending hold up time at 60 °C from 14.3 to 15 minutes. Additionally, the ramp rate was increased to 30 °C/min from 150 °C to 220 °C to accelerate the nontarget contaminant elution. The tweaked method was then applied to 23 impurity mixture analysis for separation check. Results showed 21 compounds can be resolved at baseline level using nitrogen carrier gas.

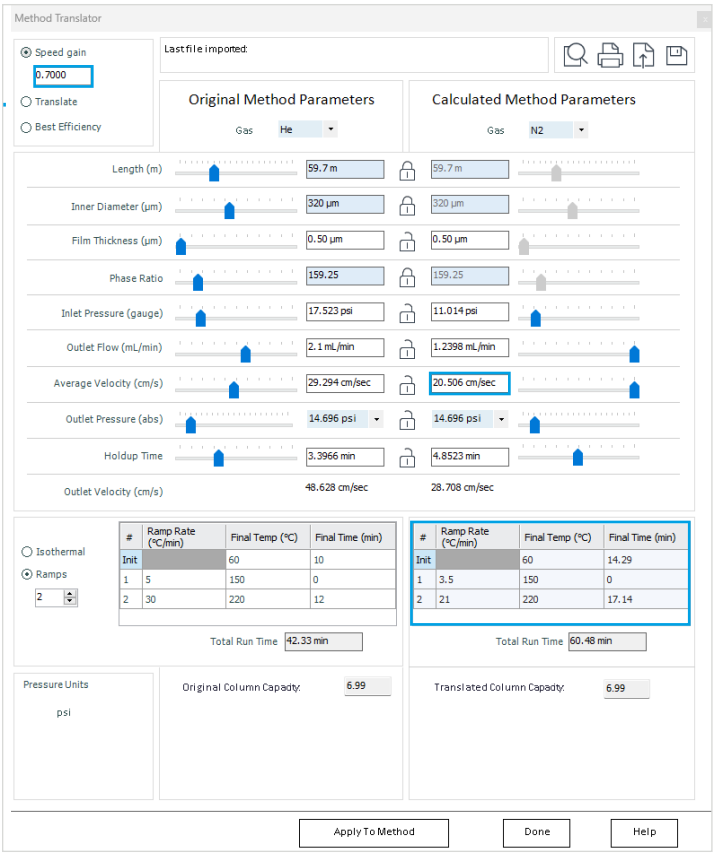


Figure 1. The nitrogen method was translated from the helium method using the method translation tool.

Chromatograms of the 23-impurity mixture on the two channels using helium, nitrogen, and hydrogen carrier gases are presented in Figure 2. Their retention time (RT) can be used for identification of impurities (RT information is shown in Table 4).

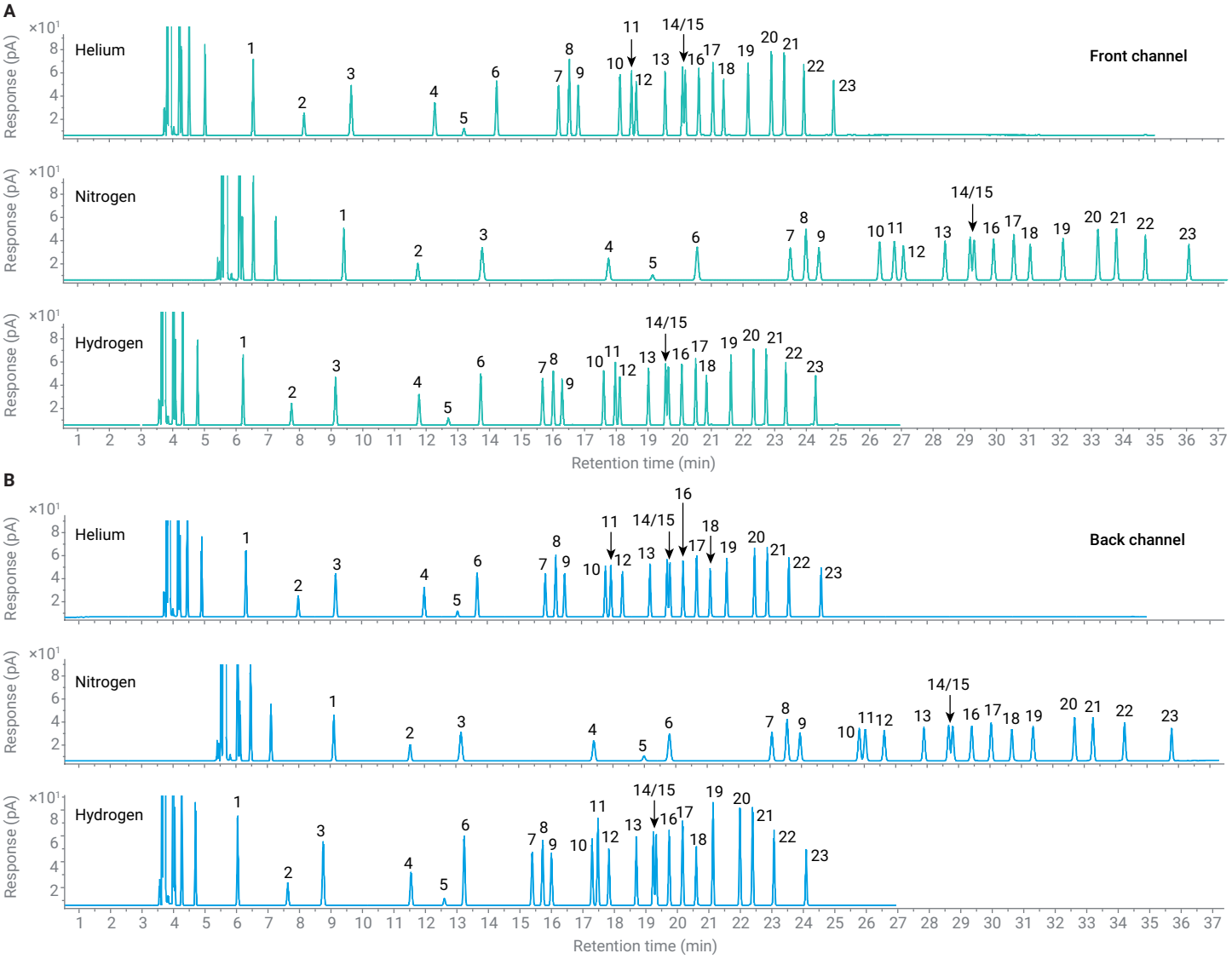


Figure 2. (A) Chromatograms of the 23-impurity mixture on the front channel using helium, nitrogen, and hydrogen carrier gases. (B) Chromatograms of 23-impurity mixture on the back channel using helium, nitrogen, and hydrogen carrier gases.

Table 4. Retention times of the 23 impurities on front and back channels using three carrier gases.

Peak No.	Compounds Name	RT-He-front (min)	RT-He-back (min)	RT-N_2-front (min)	RT-N_2-back (min)	RT-H_2-front (min)	RT-H_2-back (min)
1	*n*-Nonane	6.541	6.318	9.403	9.116	6.222	6.038
2	Benzene	8.146	7.983	11.738	11.545	7.752	7.630
3	Decane	9.634	9.173	13.768	13.161	9.142	8.764
4	Toluene	12.273	11.992	17.756	17.392	11.776	11.543
5	1,4-dioxane	13.193	13.053	19.147	18.990	12.702	12.603
6	Undecane	14.226	13.678	20.554	19.799	13.723	13.233
7	Ethylbenzene	16.179	15.846	23.496	23.060	15.676	15.390
8	*p*-Xylene	16.519	16.179	23.989	23.542	16.013	15.721
9	*m*-Xylene	16.799	16.461	24.397	23.955	16.292	16.022
10	Cumene	18.118	17.760	26.315	25.842	17.604	17.293
11	Dodecane	18.482	17.934	26.779	26.030	17.97	17.478
12	*o*-Xylene	18.632	18.301	27.064	26.635	18.111	17.827
13	Propylbenzene	19.544	19.179	28.38	27.898	19.107	18.698
14	*p*-Ethyltoluene	20.093	19.724	29.169	28.685	19.56	19.237
15	*m*-Ethyltoluene	20.18	19.813	29.296	28.813	19.646	19.326
16	*t*-Butylbenzene	20.607	20.232	29.912	29.418	20.07	19.742
17	*sec*-Butylbenzene	21.052	20.664	30.549	30.038	20.508	20.167
18	Styrene	21.388	21.097	31.067	30.696	20.848	20.600
19	Tridecane	22.162	21.621	32.102	31.373	21.62	21.133
20	1,3-Diethylbenzene	22.895	22.506	33.205	32.693	22.333	21.989
21	*n*-Butylbenzene	23.301	22.912	33.788	33.277	22.731	22.389
22	*α*-Methylstyrene	23.922	23.598	34.701	34.283	23.353	23.069
23	Phenylacetylene	24.861	24.625	36.074	35.783	24.291	24.010

Column resolution evaluation

p-Xylene check standard number one was diluted to the concentration of ~ 0.03% *m*-xylene using highly pure *p*-xylene and then separated under the three methods. The separation of *m*-xylene and *p*-xylene was used to evaluate the column resolution. ASTM D7504 requires that the distance from the valley to the baseline between two peaks should not be greater than 50% of the peak height of the lower peak. For the *m*-xylene impurity in *p*-xylene solvent, the ratio of *m*-xylene peak height versus valley-to-baseline height should be no less than 2:1. As shown in the chromatograms (Figure 3), the selected Agilent J&W HP-INNOWax column provides H/V ratio bigger than 5:1, exceeding the resolution criterion easily.

System precision

System precision following ASTM D7504 was evaluated using lab-made benzene, toluene, and *p*-xylene check standards. Ten consecutive dual-simultaneous injections of the check standards were made under each carrier gas. Representative chromatograms using helium carrier gas on two analytical channels are shown in Figure 4.

The precision of peak response and the corresponding mass concentration on both analytical channels using helium carrier gas are great with area %RSD below 1.0% for all compounds except for 1,4-dioxane and cumene due to their lower concentrations. Among all impurities, 1,4-dioxane in benzene shows the worst response precision (2.9% ~ 5.2%) on both channels. Its mass concentration was ~ 0.0022%, meaning 0.11 ng 1,4-dioxane was loaded on column for detection. The ECN of 1,4-dioxane is 3.07 indicating its absolute response factor (response/mass) is less than one-third of hydrocarbons and monocyclic aromatic solvents. The tiny amount and low response property determined its peak was small and the area precision was not as good as other compounds.

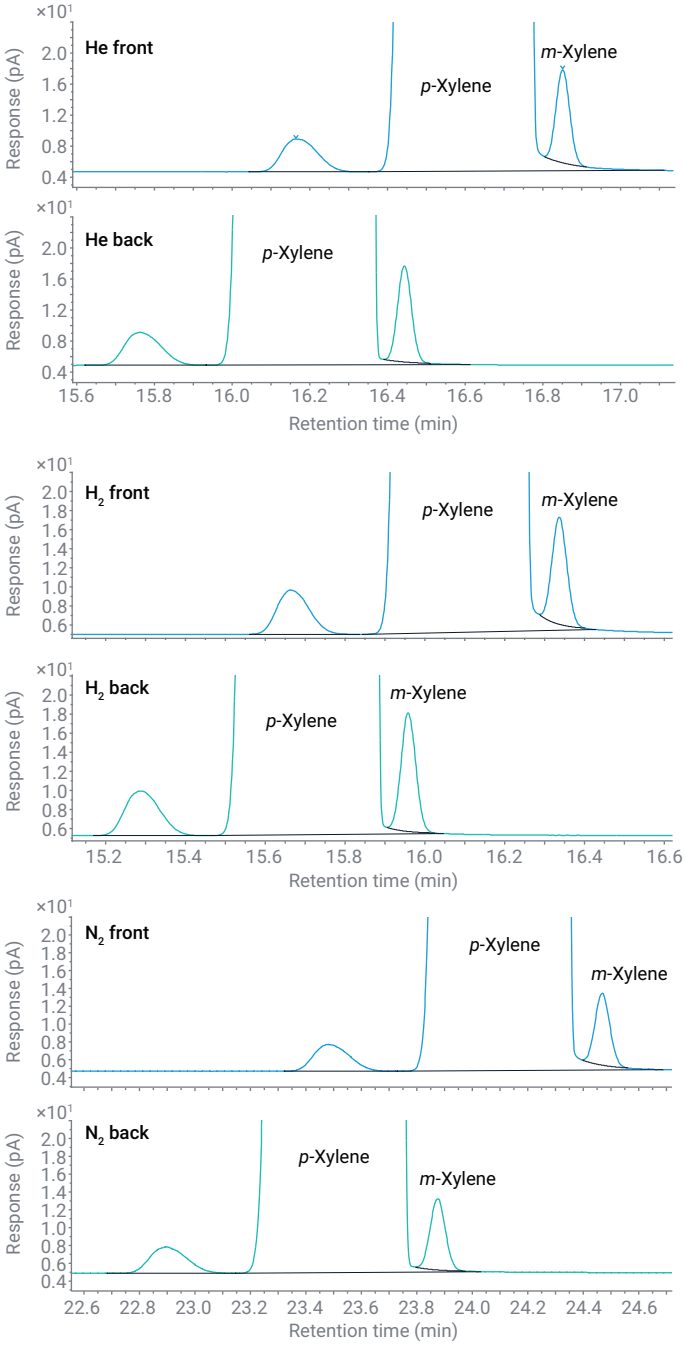


Figure 3. Resolution of *p*-xylene and *m*-xylene on dual channels using three methods.

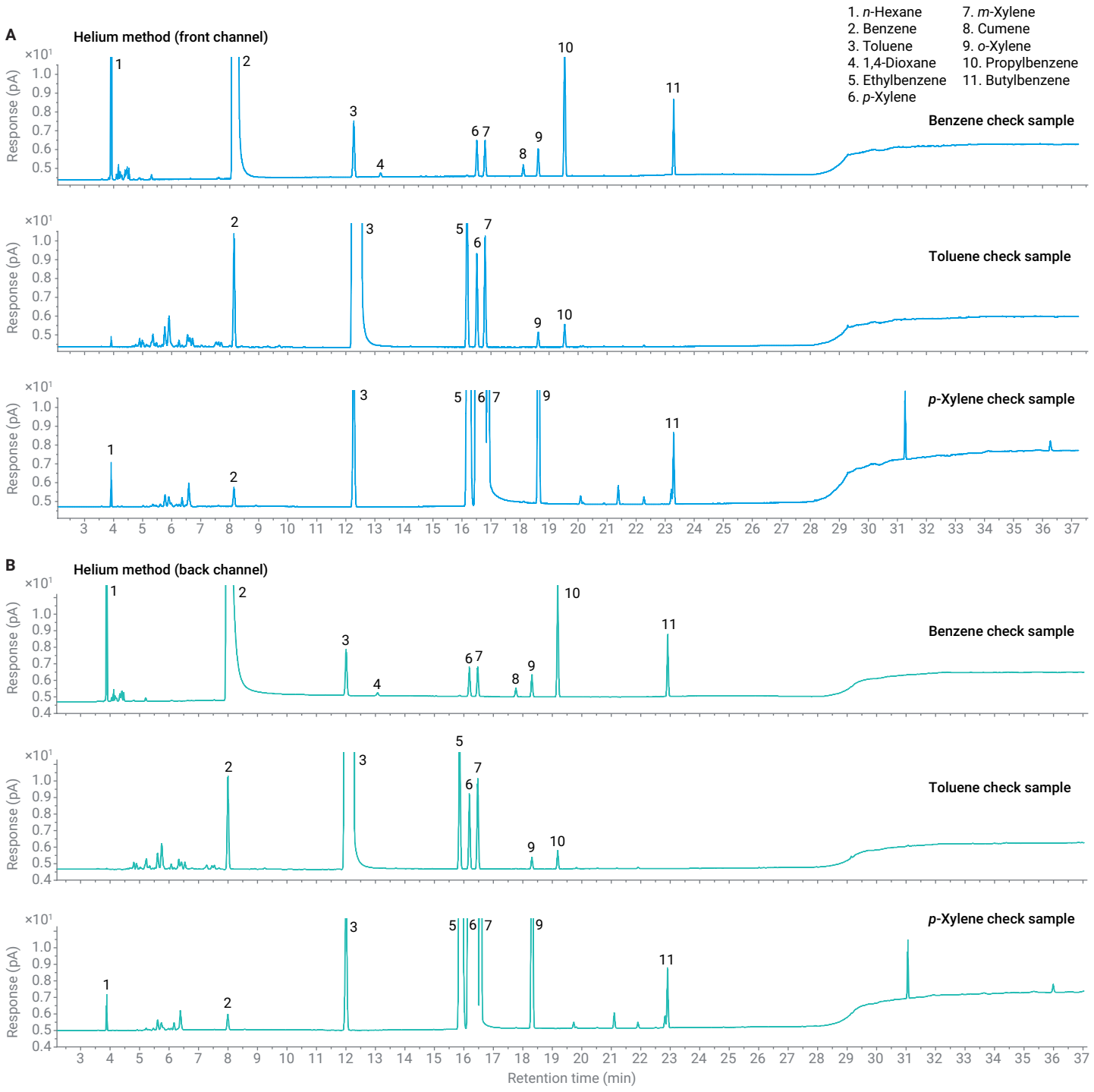


Figure 4. (A) Benzene, toluene, and *p*-xylene check standards on front channel using helium carrier gas. (B) Benzene, toluene, and *p*-xylene check standards on back channel using helium carrier gas

The retention time precision of three check standards running under helium method is shown in Table 6. The RT %RSD on the front channel ranged from 0.003 to 0.015% and the RT %RSD on the back channel was from 0.003 to 0.05%.

Nitrogen and hydrogen methods showed similar precision results as the helium methods. Chromatograms obtained using nitrogen and hydrogen carrier gas and the precision summary are shown in the Appendix.

Table 5. Impurities response and quantitation precision for benzene, toluene, and *p*-xylene check standards using helium carrier gas.

Benzene Check Standard										
	Front Channel				Back Channel				Difference of Two Channels	Reproducibility Limits(R)
Impurity	%Mass	%Mass %RSD	Area	Area %RSD	%Mass	%Mass %RSD	Area	Area %RSD		
n-C_6	0.031794	0.408	36.974	0.402	0.031695	0.355	34.135	0.544	−9.9E-05	
Benzene	99.90796	0	127,747.027	0.454	99.913267	0	117,592.951	0.652	0.005307	0.0247
Toluene	0.008925	0.267	11.288	0.546	0.009076	0.346	10.631	0.632	0.000151	0.011
1,4-Dioxane	0.002144	3.349	0.81	3.559	0.00222	5.157	0.777	5.102	7.6E-05	
p-Xylene	0.004996	0.26	6.266	0.608	0.005084	0.642	5.943	0.934	8.8E-05	
m-Xylene	0.004998	0.313	6.27	0.645	0.005089	0.567	5.912	0.921	9.1E-05	
Cumene	0.001592	1.62	1.985	1.73	0.001615	1.391	1.864	1.691	2.3E-05	
o-Xylene	0.003677	0.512	4.613	0.737	0.003735	1.01	4.339	1.223	5.8E-05	
n-Propylbenzene	0.018387	0.365	22.92	0.656	0.018692	0.47	21.579	0.907	0.000305	
n-Butylbenzene	0.009153	0.36	11.353	0.658	0.009249	0.503	10.624	0.951	9.6E-05	
Toluene Check Standard										
	Front Channel				Back Channel				Difference of Two Channels	Reproducibility Limits(R)
Impurity	%Mass	%Mass %RSD	Area	Area %RSD	%Mass	%Mass %RSD	Area	Area %RSD		
Benzene	0.015738	0.131	18.12	0.436	0.015988	0.2	18.711	0.362	0.00025	0.0022
Toluene	99.924051	0	113979.546	0.397	99.923686	0	115961.321	0.361	−0.000365	0.0131
Ethylbenzene	0.026454	0.165	29.927	0.398	0.026501	0.136	30.424	0.374	4.7E-05	0.0029
p-Xylene	0.013029	0.22	14.727	0.39	0.01305	0.217	14.982	0.435	2.1E-05	0.0029
m-Xylene	0.01564	0.157	17.679	0.432	0.01567	0.246	17.99	0.41	3E-05	0.0037
o-Xylene	0.002061	0.67	2.33	0.8	0.002074	0.878	2.381	1.037	0.000013	0.002
n-Propylbenzene	0.003027	0.618	3.401	0.745	0.00303	0.844	3.457	0.976	3E-06	0.0028
***p*-Xylene Check Standard**										
	Front Channel				Back Channel				Difference of Two Channels	Reproducibility Limits(R)
Impurity	%Mass	%Mass %RSD	Area	Area %RSD	%Mass	%Mass %RSD	Area	Area %RSD		
n-C_6	0.002626	0.697	2.993	0.817	0.002631	0.971	2.818	1.043	5E-06	0.0043
Benzene	0.002712	0.744	3.398	0.725	0.002729	0.453	3.214	0.542	1.7E-05	0.0013
Toluene	0.033612	0.128	41.658	0.428	0.033803	0.181	39.379	0.416	0.000191	0.0027
Ethyl benzene	0.245836	0.025	305.307	0.484	0.246874	0.026	285.238	0.326	0.001038	0.001
p-Xylene	99.229175	0.001	121973.152	0.482	99.22707	0	114646.657	0.342	−0.002105	0.0173
m-Xylene	0.376303	0.123	462.555	0.548	0.377201	0.12	435.817	0.377	0.000898	0.0165
o-Xylene	0.087991	0.042	108.159	0.505	0.088478	0.065	102.228	0.319	0.000487	0.0024
n-Butylbenzene	0.008862	0.182	10.771	0.575	0.008878	0.224	10.143	0.297	1.6E-05	0.0017

Table 6. Retention time (RT) and RT %RSD of three check standards in the helium method.

Benzene Check Standard				
Compounds	Front Channel		Back Channel	
	RT	RT RSD%	RT	RT RSD%
n-C_6	3.916	0.008	3.884	0.006
Benzene	8.256	0.011	8.099	0.011
Toluene	12.273	0.009	12.010	0.008
1,4-Dioxane	13.198	0.014	13.073	0.010
p-Xylene	16.515	0.005	16.191	0.005
m-Xylene	16.796	0.006	16.473	0.005
Cumene	18.114	0.005	17.769	0.004
o-Xylene	18.627	0.004	18.311	0.004
n-Propylbenzene	19.539	0.004	19.187	0.004
n-Butylbenzene	23.295	0.002	22.917	0.003
Toluene Check Standard				
Compounds	Front Channel		Back Channel	
	RT	RT RSD%	RT	RT RSD%
Benzene	8.148	0.009	7.999	0.007
Toluene	12.505	0.010	12.240	0.010
Ethylbenzene	16.177	0.005	15.859	0.005
p-Xylene	16.517	0.004	16.190	0.004
m-Xylene	16.797	0.004	16.472	0.004
o-Xylene	18.628	0.003	18.309	0.005
n-Propylbenzene	19.539	0.003	19.185	0.004
***p*-Xylene Check Standard**				
Compounds	Front Channel		Back Channel	
	RT	RT RSD%	RT	RT RSD%
n-C_6	3.917	0.010	3.884	0.012
Benzene	8.148	0.015	7.995	0.047
Toluene	12.274	0.009	12.005	0.050
Ethylbenzene	16.212	0.014	15.891	0.037
p-Xylene	16.800	0.012	16.461	0.032
m-Xylene	16.903	0.009	16.568	0.031
o-Xylene	18.638	0.006	18.315	0.026
n-Butylbenzene	23.294	0.005	22.911	0.017

Limit of detection and limit of quantitation

The method sensitivity was evaluated by running ten consecutive injections of 0.0006% benzene on both channels under three carrier gases. The LOD (with SNR at 3:1) and LOQ (SNR at 10:1) were calculated using the average SNR of benzene (Table 7). The LODs and LOQs achieved are better than their corresponding requirements of 0.0002 and 0.0006% in ASTM D7504. The sensitivity on two test channels is very close to each other under the same method. The quantitation limit of the helium method is the best due to the sharper peaks (compared to the nitrogen method) and cleaner baseline (compared to the hydrogen method).

Table 7. LODs and LOQs calculated based on the average signal to noise ratio of benzene.

Carrier Gas	He Method		N_2 Method		H_2 Method	
Channels	Front	Back	Front	Back	Front	Back
Average SNR	43:1	40.2:1	32.0:1	28.9:1	40:1	36:1
Average Area	0.838	0.818	0.722	0.725	0.758	0.717
Area %RSD	2.336	2.623	2.464	4.779	3.973	3.895
LOD (mass %)	0.000042	0.000045	0.000056	0.000062	0.000045	0.00005
LOQ (mass %)	0.00014	0.00015	0.00019	0.00021	0.00015	0.00017

Results consistency of dual-simultaneous injection

The quantification consistency of impurities in three lab-made check standards are compared between two channels. According to ASTM D7504, the dual-channel result consistency can be confirmed with a 95% probability of being correct if their difference is below the reproducibility (R) thresholds coming from ASTM D7504 ILS results. As shown in Table 5, the dual-channel quantitation difference of each probe impurity (column 10) is below the statistical R value (column 11) in the helium method except for the ethylbenzene in *p*-xylene. The ethylbenzene mass concentration in the lab-made *p*-xylene check standard is 0.245%, which has no corresponding R value in ASTM D7504 ILS research results. D7504 shows the R value for 0.0085% ethylbenzene impurity in *p*-xylene is 0.001%. The higher the impurity mass concentration, the bigger the R value. Thus, the R value for 0.245% ethylbenzene is supposed to be several times of 0.001%. This assumption can be confirmed from the R values of 0.002% for 0.0265% ethylbenzene in toluene as shown in ASTM D7504. The quantitation difference for 0.245% ethylbenzene between two channels is 0.0011%, much less than the R value for 0.0265% ethylbenzene, indicating ethylbenzene quantitation between two channels is also consistent.

The results consistency between two channels were also evaluated for the nitrogen and hydrogen methods with the same conclusion as shown in the Appendix Tables A1 and A2. The excellent quantitation consistency between the front and back analytical channels is the foundation of applying dual-channel simultaneous analysis mode to high throughput sample analysis or using one channel as a back up for another channel without calibration standards.

Results accuracy

ASTM does not recommend a reference material for determining the bias in this test method. Thus, a recovery test was made to evaluate the quantification accuracy using the described system. Eight impurities of accurate mass were added to the high pure *p*-xylene solvent, in which there is zero or very low level of impurities. Then the added impurities were measured. The recovery results based on the test values, ranging from 92 to 105%, were shown in Table 8 and Figure 5. The lowest recovery in all three methods compared to other impurities was *m*-xylene. It is due to the nonbaseline resolution of *m*-xylene impurity and *p*-xylene solvent. Seven other compounds demonstrated excellent and comparable recovery performance in three methods. The ppm level impurities were detected with satisfactory recovery indicating the 8860B GC system is a reliable platform for accurate quality control of aromatic solvents impurity.

Table 8. Recovery of added impurities for *p*-xylene.

Compound	Mass % Added	*Mass % Measured			Results Recovery (%)		
		He	N_2	H_2	He	N_2	H_2
n-C_9	0.0048	0.0048	0.0046	0.0045	98.9	96.2	92.9
Benzene	0.0048	0.0050	0.0048	0.0049	103.7	100.1	102.4
Toluene	0.0041	0.0042	0.0042	0.0042	103.9	102.9	103.1
Ethylbenzene	0.0233	0.0240	0.0240	0.0239	103.3	103.1	102.8
m-Xylene	0.0288	0.027	0.027	0.027	92.7	93.8	93.9
Cumene	0.0052	0.005	0.005	0.005	99.0	100.6	98.6
o-Xylene	0.0241	0.024	0.024	0.024	100.0	100.8	100.0
p-Diethylbenzene	0.0052	0.005	0.005	0.005	98.1	100.6	98.1

* Mass % measured is the average of dual channel results under each method.

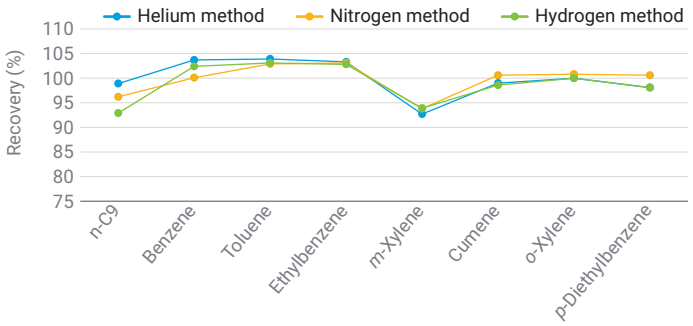


Figure 5. Recovery rate plot of added impurities for *p*-xylene.

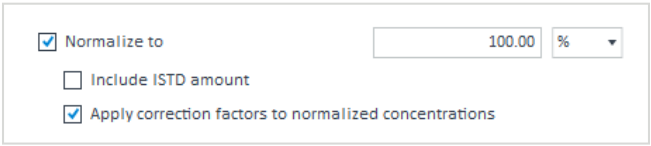
Quantification and reports by OpenLab CDS

ASTM D7504 quantitates the sample impurity by normalizing the adjusted response of each peak according to its ECN. OpenLab CDS software can easily implement peak area adjustment, normalization, and report generation by processing raw data using the preset method. The key settings made in data-processing method include:

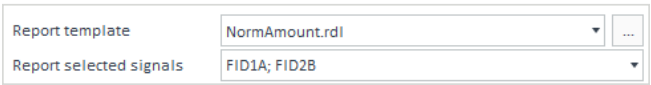
– Enabling manual factor mode in the calibration table to use the ECN of each impurity for response adjustment.

Name	Use in normalization	Mode	Manual factor
Toluene-B	☑	Manual factor	0.919500000
Toluene-F	☑	Manual factor	0.919500000
1,4-dioxane-B	☑	Manual factor	3.077400000
1,4-Dioxane-F	☑	Manual factor	3.077400000

– Enabling normalization function in calibration type setting and select **Apply correction factors to normalized concentrations** to implement adjusted area-based normalization.



– Selecting **NormAmount** template or self-defined template for normalization report generation on target signal.



With these method settings and linking the method to acquired data, a normalization report is generated upon the date processing is completed. A quantification report for benzene check standard in the front channel is shown in Figure 6 as an example.

Compounds and unknown peaks results

RT (min)	Type	Name	Group name	Area	Amount	Norm. amount (%)
3.917	VB	n-C6		36.876	36.88	0.03189
8.257	BB	Benzene		127023.695	115528.05	99.90772
12.274	BB	Toluene		11.226	10.32	0.00893
13.202	BB	1,4-Dioxane		0.762	2.34	0.00203
16.515	BB	p-Xylene		6.207	5.75	0.00498
16.796	BB	m-Xylene		6.203	5.75	0.00497
18.114	BB	Cumene		1.975	1.84	0.00159
18.627	BB	o-Xylene		4.565	4.23	0.00366
19.538	BB	n-Propylbenzene		22.803	21.27	0.01840
23.295	BB	n-Butylbenzene		11.288	10.58	0.00915
					Sum:	99.99

Groups results

Name	Group type	Total area	Amount	Norm. amount
Non-aromatics	Timed group			
non-Aromatics	Timed group (3.5 Min:16 Min)	7.734	7.73	0.00669

Figure 6. The quantification report for benzene check standard (front channel).

Conclusion

The Agilent 8860B gas chromatography system configured with two identical analytical channels are applied for impurity analysis in monocyclic aromatic solvents using three carrier gases. Each analytical channel was evaluated according to the ASTM D7504 method in terms of resolution, sensitivity, quantitation precision, and recovery with satisfactory results. The quantitation results between the two channels are consistent with each other.

- Column resolution compounds pair demonstrated good separation with H/V no less than 5:1 for 300 ppm *m*-xylene and *p*-xylene solvent.
- The LODs achieved for benzene on each analytical channel are less than 0.0001%, exceeding the 0.0002% LOD required by ASTM D7504.
- The response and mass concentration precisions of most impurities in check standards are below 1%, meeting or exceeding the precision requirements in D7504.
- Excellent recovery results, ranging from 93 to 105%, was achieved for added impurities, indicating good quantification accuracy based on the 8860B GC system.
- The quantitation difference of all probe impurities between two channels is less than the reproducibility thresholds (R), demonstrating excellent across channel consistency.

Besides great instrument performance, the Agilent OpenLab CDS software can realize ECN based normalization for easy and fast quantitation and report generation.

The 8860B dual channel GC system coupled with the OpenLab CDS software provides an accurate and reliable analysis of impurities in monocyclic aromatic solvents with satisfactory precision. Lab productivity can be improved significantly compared to the single channel analytical system.

References

1. ASTM D7504-23. Standard Test Method for Trace Impurities in Monocyclic Aromatic Hydrocarbons by Gas Chromatography and Effective Carbon Number. *ASTM International*, **2023**.
2. Scott, H. The Analysis of Monocyclic Aromatic Hydrocarbons by ASTM D7504 on the Agilent 8850 GC System. *Agilent Technologies application note*, 5994-7409EN, **2024**.
3. Zhang, Y. A Unified Method for the Analysis of Monocyclic Aromatic Solvents Using the Agilent 8860 GC System and On-Board Data Processing. *Agilent Technologies application note*, 5994-1586EN, **2022**.

Appendix

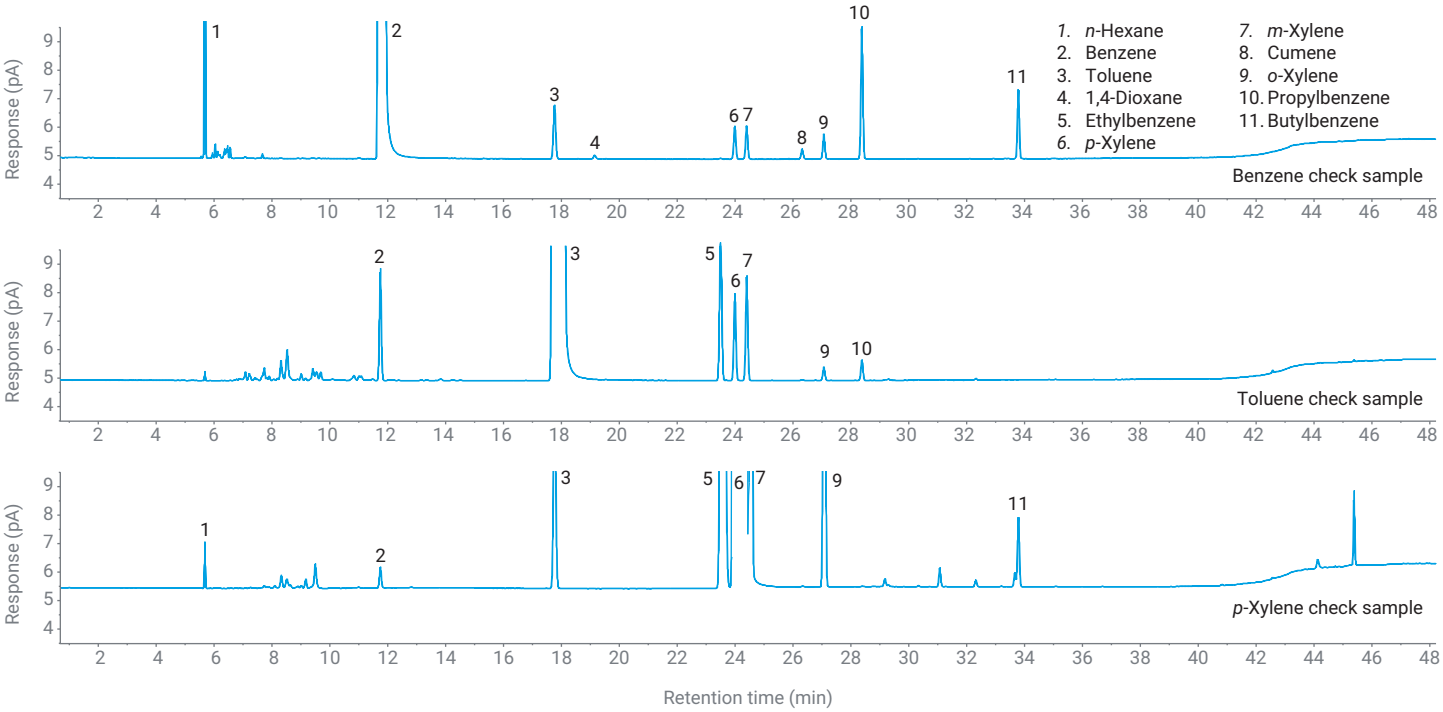


Figure A1. Benzene, toluene, and *p*-xylene check standards on front channel using nitrogen carrier gas.

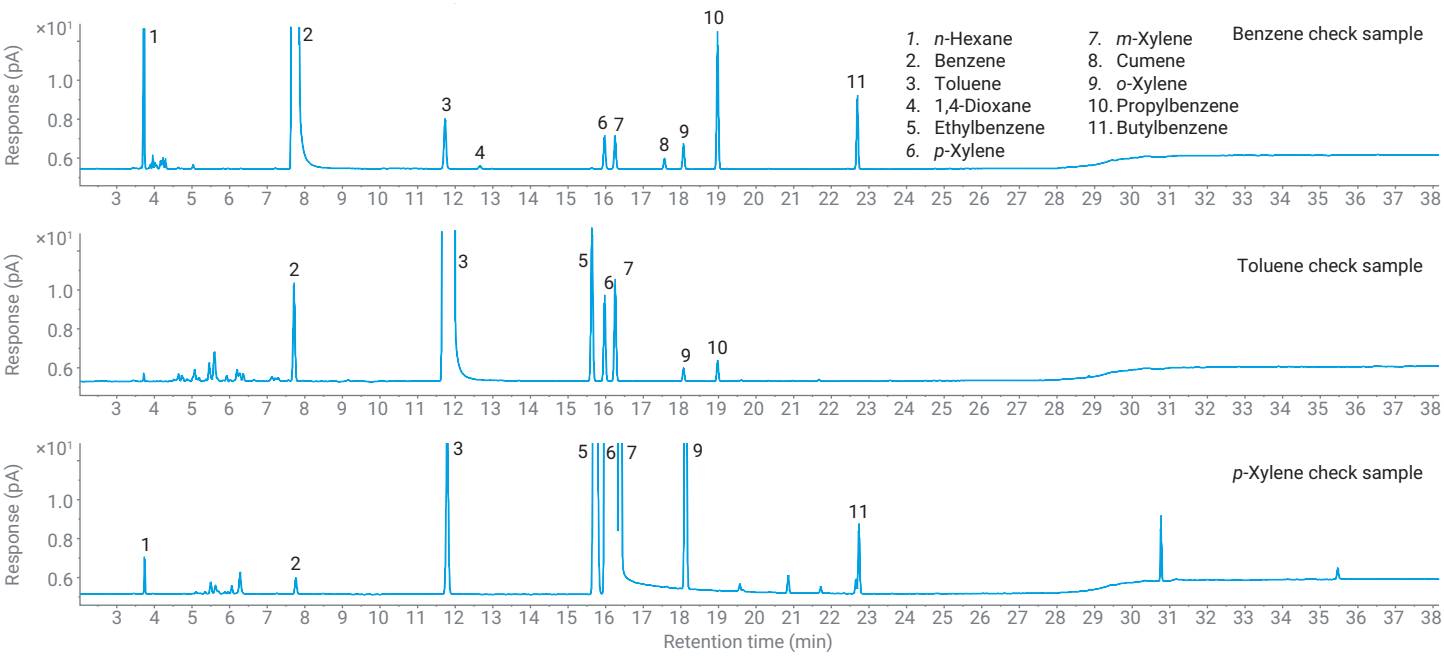


Figure A2. Benzene, toluene, and *p*-xylene check standards on front channel using hydrogen carrier gas.

Table A1. Impurities response precision in benzene, toluene, and *p*-xylene check standards using nitrogen carrier gas.

Benzene Check Standard										
	Front Channel				Back Channel				Difference of Two Channels	Reproducibility Limits (R)
Impurity	Mass%	Mass% RSD	Area	Area RSD%	Mass%	Mass% RSD	Area	Area RSD%		
n-C_6	0.030945	0.657	33.124	0.683	0.031025	0.599	32.662	0.684	−8E-05	
Benzene	99.913267	0	117,932.271	0.652	99.913796	0	115,654.795	0.699	−0.000529	0.0247
Toluene	0.009157	0.504	10.66	0.89	0.009046	0.414	10.357	0.877	0.000111	0.011
1,4-Dioxane	0.002134	4.828	0.742	5.076	0.002093	3.639	0.716	3.771	4.1E-05	
p-Xylene	0.00518	0.476	5.981	0.95	0.005123	0.741	5.818	1.17	5.7E-05	
m-Xylene	0.005188	0.791	5.991	1.336	0.005129	0.737	5.824	0.858	0.000059	
Cumene	0.001633	0.844	1.874	1.208	0.001639	1.403	1.85	1.441	−6E-06	
o-Xylene	0.0038	0.599	4.387	1.028	0.003772	0.759	4.283	1.111	2.8E-05	
Propylbenzene	0.019166	0.556	21.992	0.95	0.018928	0.48	21.36	0.938	0.000238	
Butylbenzene	0.009529	0.607	10.879	1.006	0.00945	0.724	10.611	1.092	7.9E-05	
Toluene Check Standard										
	Front Channel				Back Channel				Difference of Two Channels	Reproducibility Limits (R)
Impurity	Mass%	Mass% RSD	Area	Area RSD%	Mass%	Mass% RSD	Area	Area RSD%		
Benzene	0.015697	0.2	18.12	0.419	0.015303	0.16	17.36	0.501	3.94E-04	0.0022
Toluene	99.923097	0	114,391.735	0.471	99.922945	0	112,292.422	0.524	1.52E-04	0.0131
Ethylbenzene	0.026886	0.108	30.357	0.532	0.027108	0.151	30.172	0.556	−0.000222	0.0029
p-Xylene	0.013231	0.164	14.94	0.561	0.013321	0.243	14.827	0.504	−9E-05	0.0029
m-Xylene	0.015919	0.215	17.974	0.562	0.016052	0.197	17.866	0.42	−0.000133	0.0037
o-Xylene	0.002093	1.467	2.364	1.624	0.002121	1.626	2.361	1.884	−2.8E-05	0.002
n-Propylbenzene	0.003077	0.58	3.453	0.697	0.00315	0.858	3.485	1.155	−7.3E-05	0.0028
***p*-Xylene Check Standard**										
	Front Channel				Back Channel				Difference of Two Channels	Reproducibility Limits (R)
Impurity	Mass%	Mass% RSD	Area	Area RSD%	Mass%	Mass% RSD	Area	Area RSD%		
n-C_6	0.002571	0.879	2.718	0.794	0.002583	0.88	2.856	1.241	−1.20E-05	0.0043
Benzene	0.002684	0.51	3.121	0.74	0.00269	0.937	3.272	1.493	−6.00E-06	0.0013
Toluene	0.033585	0.218	38.62	0.851	0.033417	0.122	40.195	0.751	0.000168	0.0027
Ethylbenzene	0.247285	0.025	282.044	0.774	0.246304	0.031	293.827	0.706	0.000981	0.001
p-Xylene	99.238055	0.002	113,187.456	0.791	99.234597	0	118,381.161	0.718	0.003458	0.0173
m-Xylene	0.376102	0.543	428.981	1.243	0.377082	0.101	449.835	0.642	−0.00098	0.0165
o-Xylene	0.088837	0.075	101.324	0.801	0.088327	0.053	105.368	0.682	0.00051	0.0024
n-Butylbenzene	0.00902	0.3	10.173	0.817	0.008986	0.24	10.6	0.913	3.40E-05	0.0017

Table A2. Impurities response precision in benzene, toluene, and *p*-xylene check standards using hydrogen carrier gas.

Benzene Check Standard										
Impurity	Front Channel				Back Channel				Difference of Two Channels	Reproducibility Limits (R)
	Mass%	Mass% RSD	Area	Area RSD%	Mass%	Mass% RSD	Area	Area RSD%		
n-C_6	0.02997	0.621	31.931	1.237	0.029843	0.565	30.028	0.628	0.000127	
Benzene	99.904905	0.001	117,028.727	0.736	99.907062	0	110,530	0.359	−0.002157	0.0247
Toluene	0.009356	0.394	10.841	0.639	0.009212	0.395	10.081	0.48	0.000144	0.011
1,4-Dioxane	0.002477	2.937	0.847	2.989	0.002246	3.088	0.734	2.94	0.000231	
p-Xylene	0.005357	0.69	6.156	0.614	0.005266	0.508	5.716	0.653	9.1E-05	
m-Xylene	0.005377	0.617	6.179	0.559	0.005278	0.633	5.728	0.722	9.9E-05	
Cumene	0.001722	1.144	1.967	1.295	0.001695	0.861	1.828	0.963	2.7E-05	
o-Xylene	0.003959	0.629	4.55	0.679	0.00388	0.52	4.211	0.627	7.9E-05	
Propylbenzene	0.019965	0.736	22.799	0.639	0.019564	0.554	21.101	0.668	0.000401	
Butylbenzene	0.00996	0.946	11.317	0.96	0.009792	0.539	10.508	0.652	0.000168	
Toluene Check Standard										
Impurity	Front Channel				Back Channel				Difference of Two Channels	Reproducibility Limits (R)
	Mass%	Mass% RSD	Area	Area RSD%	Mass%	Mass% RSD	Area	Area RSD%		
Benzene	0.015375	0.74	17.831	1.405	0.015102	0.752	16.678	0.823	2.73E-04	0.0022
Toluene	99.922293	0	114,619.152	0.99	99.9226	0	1,09153	0.481	−3.07E-04	0.0131
Ethylbenzene	0.027282	0.357	31.038	1	0.027268	0.348	29.542	0.644	1.4E-05	0.0029
p-Xylene	0.01345	0.465	15.302	0.961	0.013394	0.336	14.512	0.582	5.6E-05	0.0029
m-Xylene	0.016169	0.341	18.395	1.026	0.016219	0.546	17.571	0.798	−5E-05	0.0037
o-Xylene	0.002212	2.805	2.516	3.015	0.002186	2.964	2.368	2.833	0.000026	0.002
n-Propylbenzene	0.003219	1.264	3.639	1.115	0.003231	3.479	3.401	1.215	−1.2E-05	0.0028
***p*-Xylene Check Standard**										
Impurity	Front Channel				Back Channel				Difference of Two Channels	Reproducibility Limits (R)
	Mass%	Mass% RSD	Area	Area RSD%	Mass%	Mass% RSD	Area	Area RSD%		
n-C_6	0.002232	1.022	2.459	1.129	0.002407	0.489	2.398	1.076	−1.75E-04	0.0043
Benzene	0.002439	0.47	2.954	1.033	0.002565	0.538	2.81	1.195	−1.26E-04	0.0013
Toluene	0.032358	0.218	38.763	0.869	0.032849	0.16	35.597	0.972	−0.000491	0.0027
Ethylbenzene	0.248691	0.016	295.476	0.928	0.247325	0.071	265.823	1.039	0.001366	0.001
p-Xylene	99.225286	0.001	117,891.859	0.933	99.215055	0.006	1,06636	1.088	0.010231	0.0173
m-Xylene	0.378024	0.197	449.142	1.032	0.390048	1.702	419.274	2.615	−0.012024	0.0165
o-Xylene	0.090252	0.075	107.23	1.04	0.08917	0.063	95.839	1.04	0.001082	0.0024
n-Butylbenzene	0.009438	0.153	11.087	0.982	0.009155	0.268	9.73	0.915	2.83E-04	0.0017

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