# Tools I Can't Live Without:
# Speed Up Method Development and Translation, Essentials for GC and GC/MS Users

Michelle Misselwitz, Julie Kowalski, Jack Cochran, Becca Stevens

michelle.misselwitz@restek.com

# *We need a new method developed… YESTERDAY!*

***You have*:**
Analyte list

***You need:***
GC column and instrument conditions

*Speed Up and Simplify GC Method Development With*

# Restek's *EZGC*® Online Suite


New! *EZGC*® Method Translator and Flow Calculator

*EZGC*® Chromatogram Modeler

# *EZGC*® Chromatogram Modeler

Send Us Your Feedback!

Enter compound names, synonyms, or CAS #s.

**Examples:**
1,4-dioxane
acetaldehyde, ethanol and isopropyl alcohol

I need to paste a list. Show me a list box.

Welcome to the **Restek *EZGC*® Chromatogram Modeler**, the easiest way to jump-start your method development! To get started, enter the compounds you wish to separate into the field above. To paste a list, first click the link "I need to paste a list" underneath the input field.

**Browser requirements**

To get the best results from the *EZGC*® modeler, we recommend one of the following browsers:

- Firefox (desktop or Android tablet)
- Chrome (Windows or Mac desktop or Android tablet)
- IE 8 or IE 9 or above (Windows desktop)
- Safari (desktop or iPad tablet)
- Opera (desktop or mobile)

## Learn *EZGC*® in 5 Minutes!

**Find out how easy it is to get started with the EZGC® app in this brief screencast.**

Watch the Video

## It's Easy, but Powerful!

**Restek Innovations Laboratory Manager Chris English goes into detail about how to get the most out of the EZGC modeler.**

Watch the Video

## My *EZGC*® Models

Untitled
*1,1,1,2-Tetrachloroethane, 1,1,1-Trichloroethane, 1,1,2-Trichloroethane, 1,1-Dichloroethene, 1,2,4-Trichlorobenzene...*
Dec 14, 2012

View/edit full list

# EZGC® Chromatogram Modeler

Send Us Your Feedback!

Enter a compound name, synonym or CAS #, one per line.

Go

Show me the standard entry field.

2,4'-DDD[x], 2,4'-DDE[x], 2,4'-DDT[x], 4,4'-DDD[x], 4,4'-DDE[x], 4,4'-DDT[x], 4,4'-Dibromobiphenyl[x], Captan [x], Carbophenothion[x], Chlorobenzilate[x], Decachlorobiphenyl[x], Dibutyl chlorendate[x], Dicofol[x], Dieldrin[x], Endosulfan I[x], Endosulfan II[x], Endosulfan sulfate[x], Endrin[x], Endrin aldehyde[x], Endrin ketone[x], Heptachlor epoxide[x], Isodrin[x], Kepone[x], Methoxychlor[x], Mirex[x], Show All...

The following compounds were not found:

a-chlordane[x]

acifluorfen me[x]

γ chlordane[x]

[Clear All]

**Need more help?**

Send this list to Restek Technical Service with your questions.

## Untitled. Click here to edit.

*Click title to edit*

| Peaks | Ret. Time ($t_R$) | Res. ($R_S$) | Peak Width |
|---|---|---|---|
| 1. Isodrin | 30.21 | 8.31 | 0.10 |
| 2. 4,4'-Dibromobiphenyl | 31.05 | -- | 0.10 |
| 3. Heptachlor epoxide | 31.05 | -- | 0.10 |
| 4. 2,4'-DDE | 32.14 | 3.58 | 0.10 |
| 5. Captan | 32.49 | 3.58 | 0.10 |
| 6. Endosulfan I | 33.00 | 1.02 | 0.10 |
| 7. cis-Nonachlor | 33.10 | 1.02 | 0.10 |
| 8. 4,4'-DDE | 34.08 | 2.51 | 0.10 |
| 9. Dieldrin | 34.33 | 2.14 | 0.10 |
| 10. 2,4'-DDD | 34.55 | 2.14 | 0.10 |
| 11. Perthane | 35.01 | 3.97 | 0.10 |
| 12. Endrin | 35.39 | 3.97 | 0.10 |
| 13. 2,4'-DDT | 35.83 | 4.12 | 0.10 |
| 14. trans-Nonachlor | 36.29 | 1.63 | 0.10 |
| 15. Kepone | 36.46 | 0.13 | 0.11 |
| 16. Chlorobenzilate | 36.47 | 0.13 | 0.10 |
| 17. 4,4'-DDD | 36.76 | 2.94 | 0.10 |
| 18. Endosulfan II | 37.13 | 1.98 | 0.10 |
| 19. Carbophenothion | 37.34 | 1.98 | 0.10 |
| 20. Endrin aldehyde | 37.70 | 3.26 | 0.10 |
| 21. 4,4'-DDT | 38.04 | 3.26 | 0.10 |
| 22. Endosulfan sulfate | 39.11 | 10.60 | 0.10 |
| 23. Methoxychlor | 40.42 | 3.10 | 0.10 |
| 24. Dibutyl chlorendate | 40.73 | 1.94 | 0.10 |
| 25. Endrin ketone | 40.92 | 1.56 | 0.11 |
| 26. Dicofol | 41.09 | 1.56 | 0.10 |
| 27. Mirex | 42.69 | 13.10 | 0.11 |
| 28. cis-Permethrin | 44.14 | 4.07 | 0.10 |
| 29. trans-Permethrin | 44.54 | 4.07 | 0.10 |
| 30. Decachlorobiphenyl | 47.47 | 29.80 | 0.10 |

*Not found: a-chlordane, acifluorfen me, γ chlordane*

### Product Suggestions

Rtx®-PCB Columns
cat.# 13223
$537.0/ea.
Qty: 1

Add To Cart

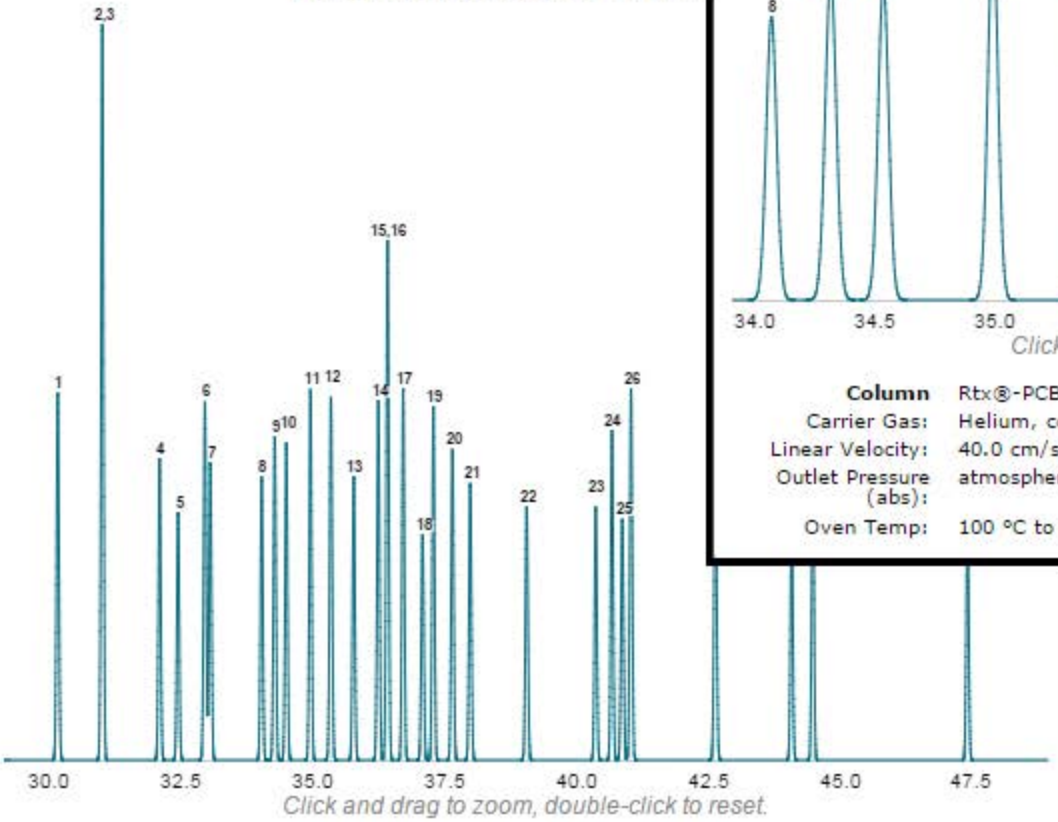
### My EZGC® Models

Untitled
*1,1,1,2-Tetrachloroethane, 1,1,1-Trichloroethane, 1,1,2-Trichloroethane, 1,1-Dichloroethene, 1,2,4-Trichlorobenzene...*
Dec 14, 2012

View/edit full list

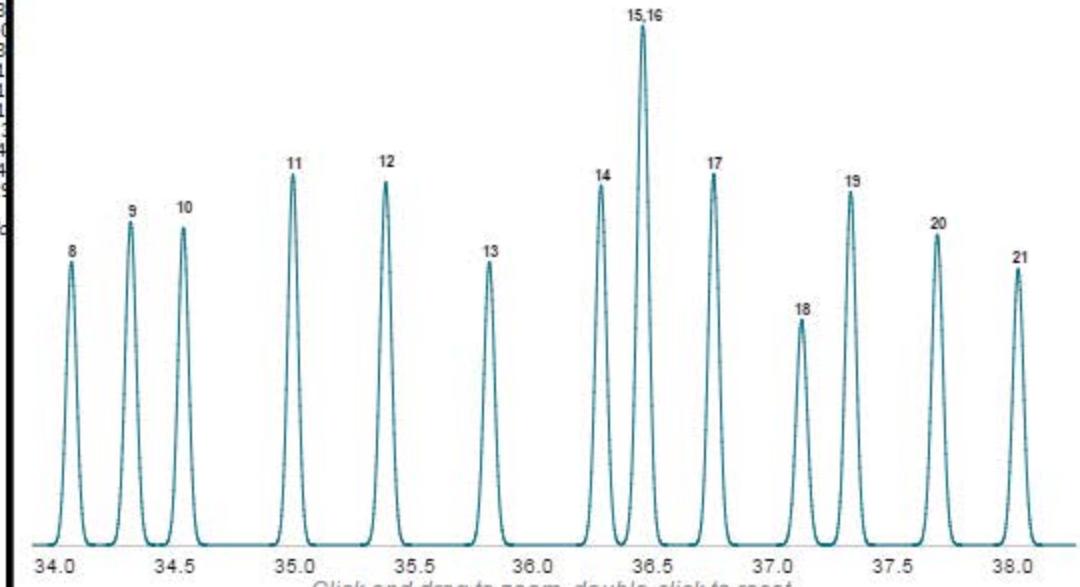
| | | | |
|---|---|---|---|
| 14. trans-Nonachlor | | 36.29 | 1 |
| 15. Kepone | | 36.46 | 0 |
| 16. Chlorobenzilate | | 36.47 | 0 |
| 17. 4,4'-DDD | | 36.76 | 2 |
| 18. Endosulfan II | | 37.13 | 1 |
| 19. Carbophenothion | | 37.34 | 1 |
| 20. Endrin aldehyde | | 37.70 | 3 |
| 21. 4,4'-DDT | | 38.04 | 3 |
| 22. Endosulfan sulfate | | 39.11 | 10 |
| 23. Methoxychlor | | 40.42 | 3 |
| 24. Dibutyl chlorendate | | 40.73 | 1 |
| 25. Endrin ketone | | 40.92 | 1 |
| 26. Dicofol | | 41.09 | 1 |
| 27. Mirex | | 42.69 | 13 |
| 28. cis-Permethrin | | 44.14 | 4 |
| 29. trans-Permethrin | | 44.54 | 4 |
| 30. Decachlorobiphenyl | | 47.47 | 29 |

*Not found: a-chlordane, acifluorfen me, γ chlo*




*Click and drag to zoom, double-click to reset.*

| | |
|---|---|
| **Column** | Rtx®-PCB, 30 m, 0.25 mm ID, 0.25 µm (cat.# 13223) |
| Carrier Gas: | Helium, constant flow @ 1.68 mL/min |
| Linear Velocity: | 40.0 cm/sec |
| Outlet Pressure (abs): | atmospheric pressure |
| Oven Temp: | 100 °C to 310 °C @ 4.0 °C/min |




*Click and drag to zoom, double-click to reset.*

| | |
|---|---|
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# *We need a new method developed… YESTERDAY!*

***You have*:**
Analyte list
GC column

***You need:***
GC instrument conditions

# We need to know…

Flow rate

Oven program

Accurate column length

Initial oven temperature

Splitless hold time

# Optimal Flow for GC

SOF EOF

# Optimal Flow for GC

## SOF

**S**peed
**O**ptimized
**F**low

## EOF

**E**fficiency
**O**ptimized
**F**low

# Theory of Fast Capillary Gas Chromatography – Part 3: Column Performance *vs.* Gas Flow Rate

**Leonid M. Blumberg**[1)]

Fast GC Consulting, PO Box 585, Hockessin, DE 19707, USA

J. High Resol. Chromatogr. **1999**, 22, (7) 403-413

Ms received: June 2, 1998; accepted: October 15, 1998

***Key Words:*** *Constant length optimization; constant efficiency optimization; efficiency-optimized flow rate; fast GC; film inefficiency factor; high pressure drop; speed-optimized flow rate*

## Speed-Optimized Flow and Efficiency-Optimized Flow

### Summary

**At the high pressure drop required for the fast analysis of complex mixtures, the equations for the column plate height, H, and plate duration, Q, as functions of the carrier gas velocity, $\bar{u}$, differ substantially from the equations for the same quantities expressed via the carrier gas flow rate, *F*. While $\bar{u}$ as an independent pneumatic variable is more convenient for the theoretical studies, *F* is a more convenient as a control parameter in practical applications. Equations for H *vs.* $\bar{u}$ and for Q *vs.* $\bar{u}$ from Parts 1 and 2 are transformed here into expressions for H *vs.* *F* and Q *vs.* *F*. An efficiency-optimized flow rate (EOF) and a speed-optimized flow rate (SOF) are found. Expressions for these two quantities are considerably simpler than their velocity-based counterparts. In particular, SOF does not depend on column length, film thickness, and pressure drop.**

### 1 Introduction

This report continues the study [1, 2] of the speed-separation performance of a capillary column having an **arbitrary film thickness** and operating at an **arbitrary pressure drop**.

At a low pressure drop, the structure of the equations for the plate height, **h**, and plate duration, **q**, does not depend on the type of the independent pneumatic variable. Thus,

$$\mathbf{h} = \frac{b}{w} + c\,w, \qquad \mathbf{q} = \frac{b}{w^2} + c$$

are, respectively, Van Deemter and Purnell [5, 6] equations in which the independent variable *w* can be either $\bar{u}$ or *F* (or the column pressure drop) while *b* and *c* are the coefficients whose values do not change with the change in the value of *w*.

At the high pressure drop, however, the structure of the expression for both the plate height, **H**, and the plate duration, **Q**, depends on the selection of the independent pneumatic variable. Thus, for example, as a function of $\bar{u}$, **H** can be expressed as (see Part 1)

$$\mathbf{H} = \frac{B}{\bar{u}^2} + C_1\bar{u}^2 + C_2\bar{u}$$

Journal of Chromatography A, 1218 (2011) 8722–8723

Contents lists available at SciVerse ScienceDirect

Journal of Chromatography A

journal homepage: www.elsevier.com/locate/chroma

Discussion

# Plate height formula widely accepted in GC is not correct

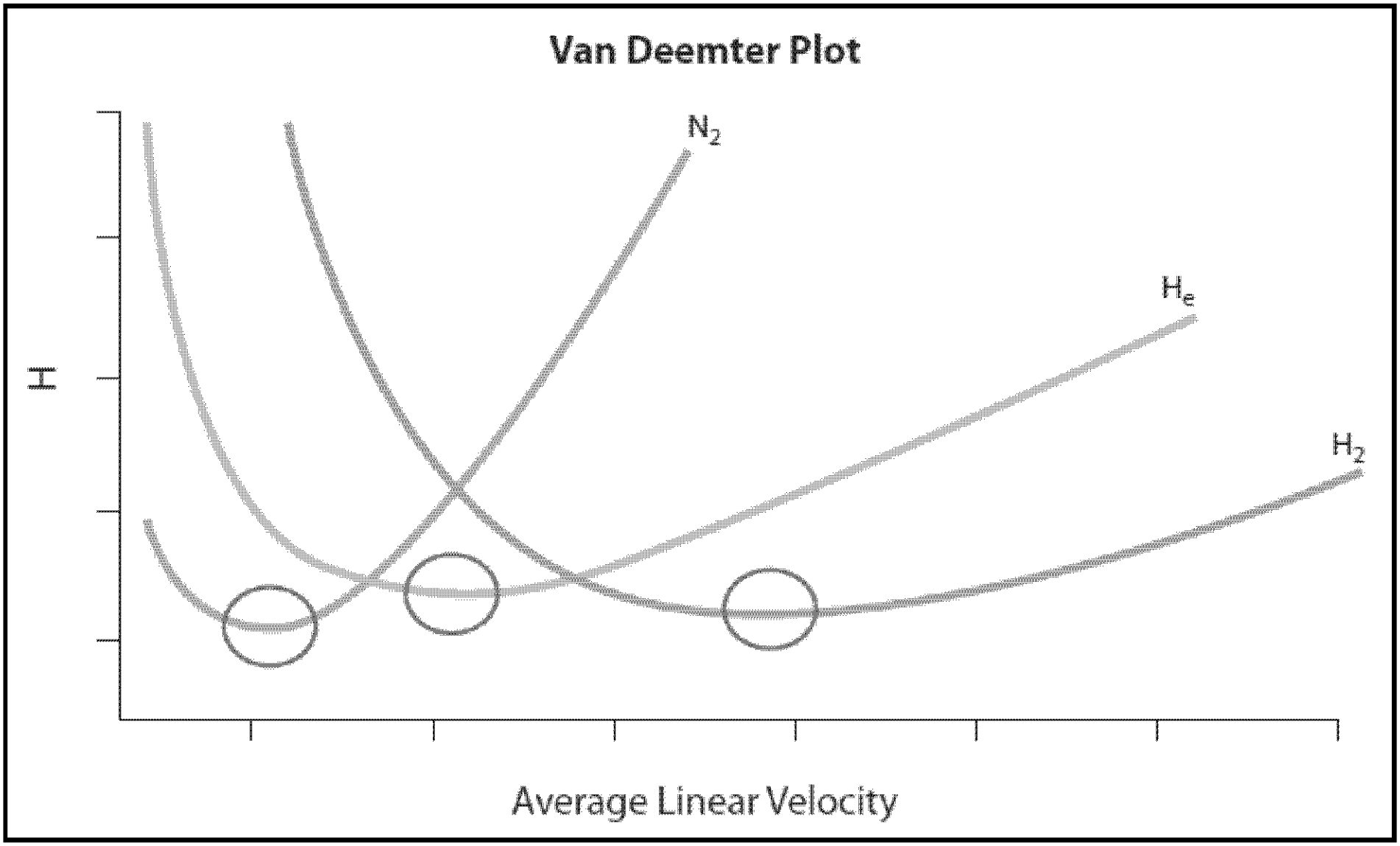
Leonid M. Blumberg

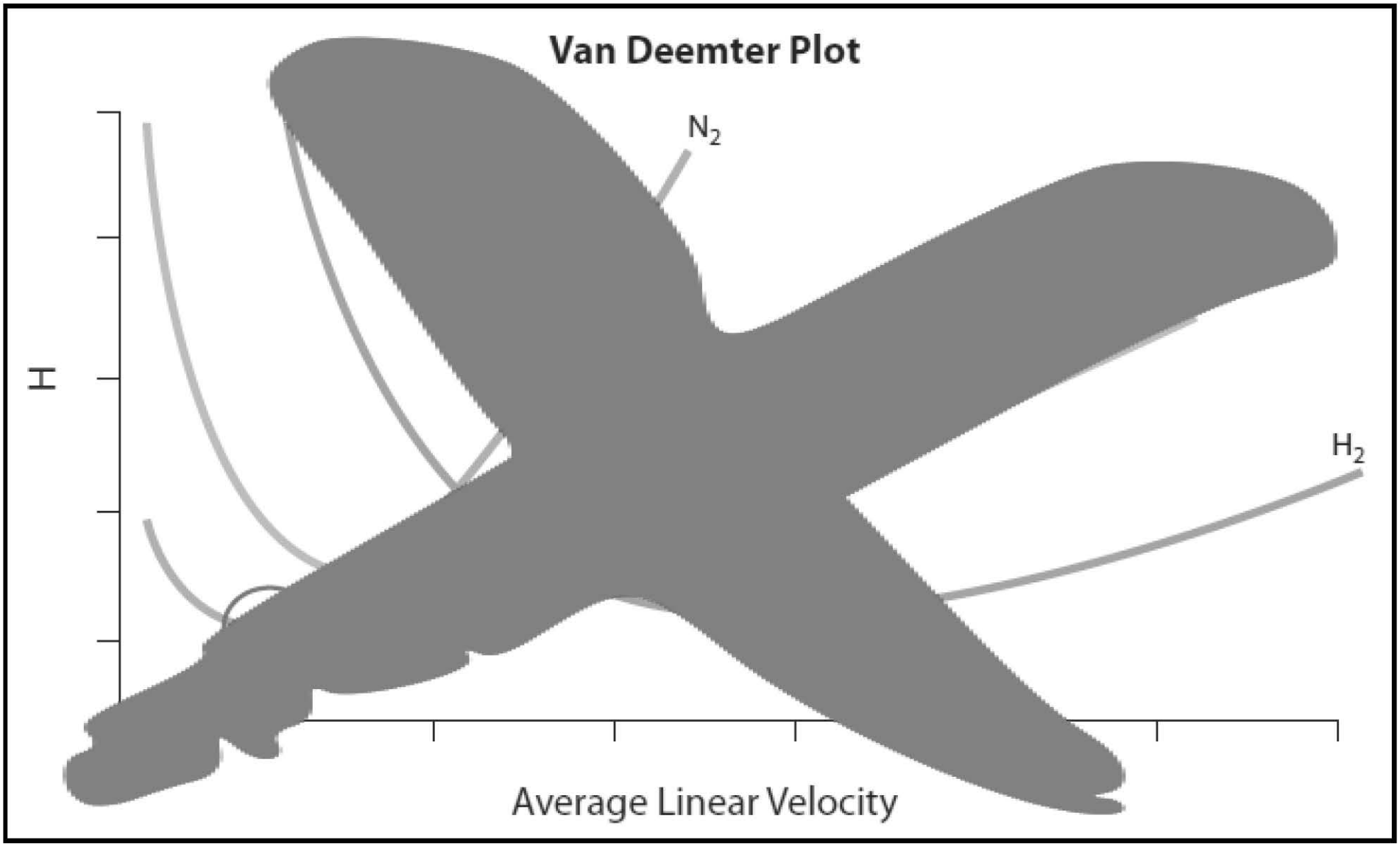
*Fast GC Consulting, PO Box 1243, Wilmington, DE 19801, USA*

*Dear Editor,*

I would like to bring to attention of the readers of your Journal that

- widely accepted formula for a column plate height ($H$) in GC is incorrect, and that
- carrier gas average velocity ($\bar{u}$) is not the best variable for describing $H$ as a function of a gas flow in GC columns.


Van Deemter Plot
N2
He
H2
H
Average Linear Velocity


Van Deemter Plot
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H2
H
Average Linear Velocity

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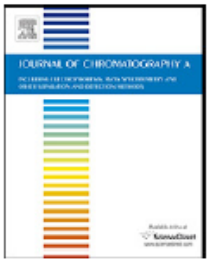

Discussion

# Plate height formula widely accepted in GC is not correct

Leonid M. Blumberg

*Fast GC Consulting, PO Box 1243, Wilmington, DE 19801, USA*

Suggests optimal FLOW rate for GC, not optimal average velocity…

*Dear Editor,*

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- widely accepted formula for a column plate height ($H$) in GC is incorrect, and that
- carrier gas average velocity ($\bar{u}$) is not the best variable for describing $H$ as a function of a gas flow in GC columns.

# Optimal Flow for GC

## SOF

**S**peed **O**ptimized **F**low

Column ID × constant

Helium
8 x column ID
8 x 0.25 = 2.0 mL/min

Hydrogen
10 x column ID
10 x 0.25 = 2.5 mL/min

## EOF

**E**fficiency **O**ptimized **F**low

$$\frac{SOF}{\sqrt{2}}$$

Helium
2.0 / $\sqrt{2}$ = 1.4 mL/min

Hydrogen
2.5 / $\sqrt{2}$ = 1.8 mL/min

# Optimal Flow for GC

## SOF

**S**peed **O**ptimized **F**low

Helium, 0.25 mm ID

**2.0 mL/min**

## EOF

**E**fficiency **O**ptimized **F**low

Helium, 0.25 mm ID

**1.4 mL/min** 

- ✓ Considerably simpler than velocity-based
- ✓ SOF does not depend on column length, film thickness, and pressure drop

# We need to know…

Flow rate ✓

Oven program

Accurate column length

Initial oven temperature

Splitless hold time

# Optimal Heating Rate in Gas Chromatography

L. M. Blumberg,[1] M. S. Klee[2]
[1] *Fast GC Consulting, P.O. Box 585, Hockessin, DE 19707, USA*
[2] *Agilent Technologies, 2850 Centerville Road, Wilmington, DE 19808, USA*

Received 8 June 2000; accepted 15 September 2000

J. Microcolumn Separations, 12 (9) 508-514 (2000)

$10 / t_M$

**Abstract:** Several optimization criteria for column heating rate in temperature programmed gas chromatography (GC), under different optimization constraints are identified. Applying these criteria to experimental data, it is shown that when column pressure drop is high, the optimum heating rate for *n*-alkanes and pesticides in a column with a silicone stationary phase of a typical thickness is about 10°C per void time. This heating rate is recommended as a default for all temperature programs in capillary GC.  J Micro Sep 12: 508–514, 2000

**Key words:** *gas chromatography; optimal heating rate; separation-speed tradeoff*

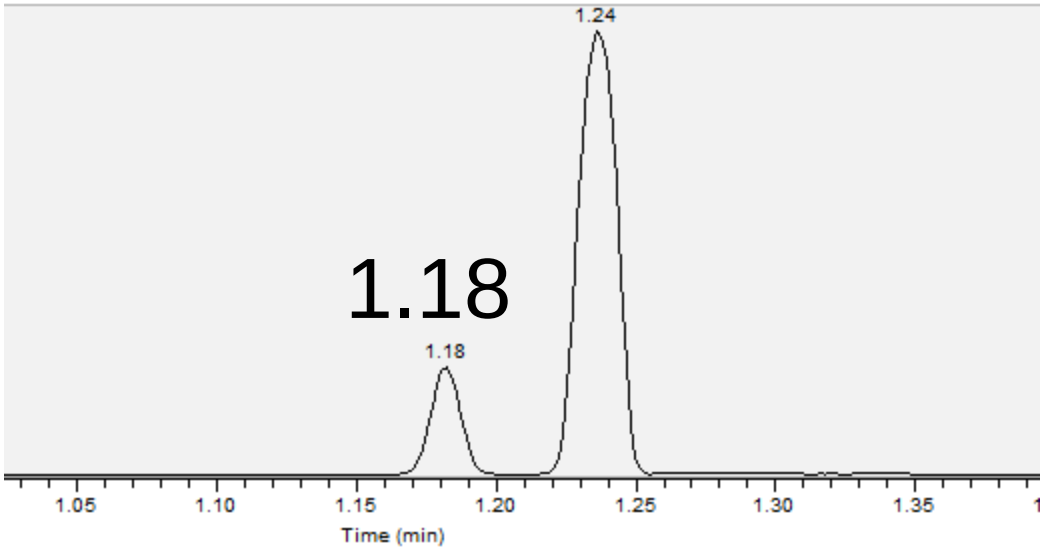
# Optimal Heating Rate for GCC

- Adequate separation of a required number of solutes in the shortest time
  - Maximizing peak capacity
  - Minimizing analysis time
- NOT aimed specifically at separating specific pairs of solutes

$$\frac{10°C}{t_M}$$

Air injection
100 split, 0.1 µL
Scan 25-100

# Optimal Heating Rate for GCC




$$\frac{10°C}{t_M} \rightarrow \frac{10°C}{1.18\ min} = 8.5°C/min$$

# We need to know…

Flow rate ✓

Oven program ✓

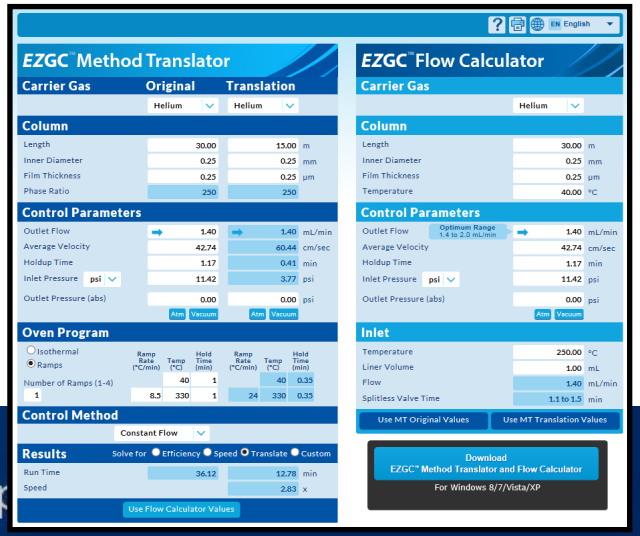
Accurate column length

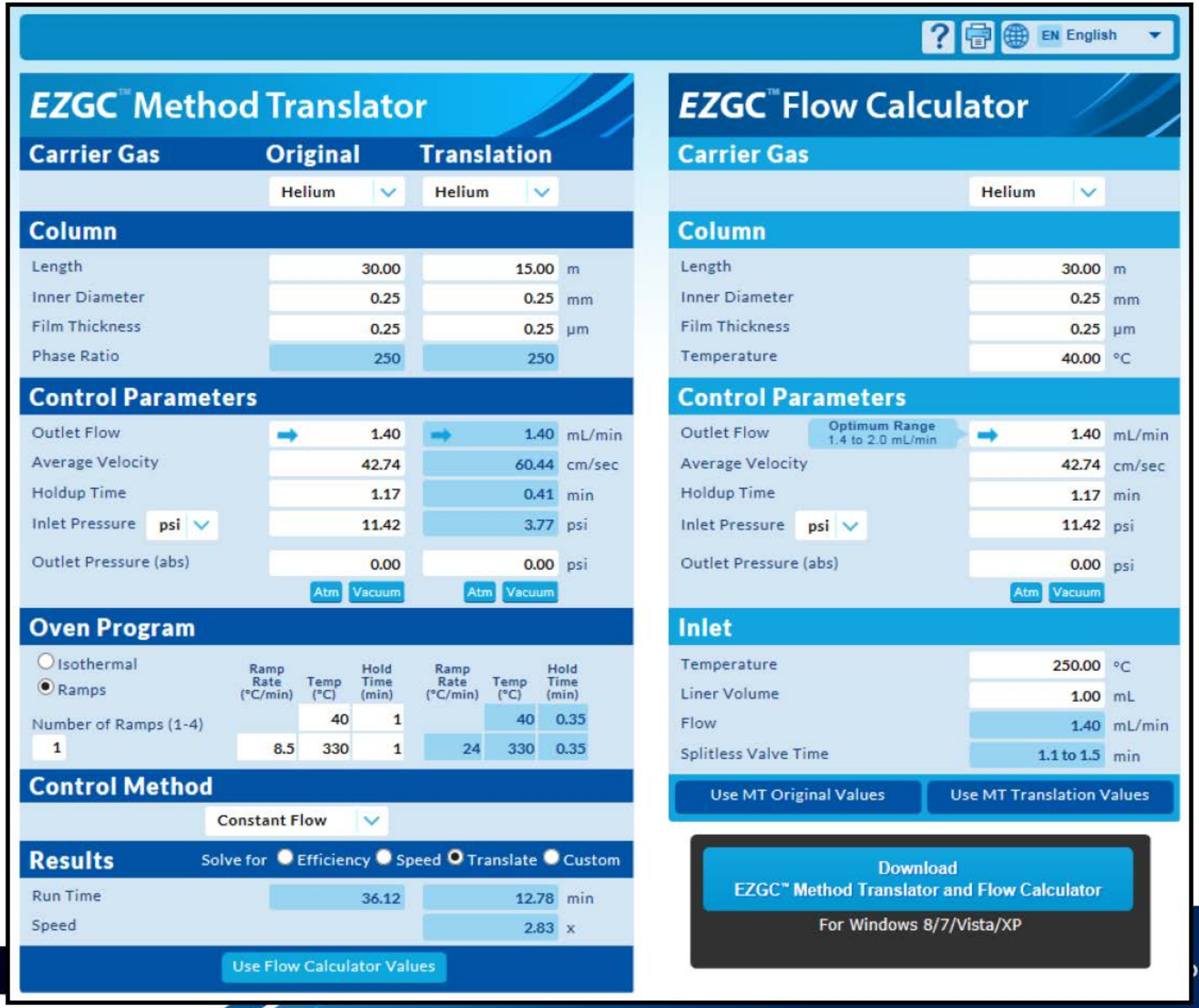
Initial oven temperature

Splitless hold time

# *EZ*GC™ Method Translator and Flow Calculator

- http://www.restek.com/ezgc-mtfc
- Available in a web-based version
- Or, download the app from the link above
- Windows 8 – 7 – Vista – XP




EN English
EZGC™ Method Translator
Carrier Gas
Original
Translation
Helium
Helium
Column
Length
30.00
15.00
m
Inner Diameter
0.25
0.25
mm
Film Thickness
0.25
0.25
µm
Phase Ratio
250
250
Control Parameters
Outlet Flow
1.40
1.40
mL/min
Average Velocity
42.74
60.44
cm/sec
Holdup Time
1.17
0.41
min
Inlet Pressure
psi
11.42
3.77
psi
Outlet Pressure (abs)
0.00
0.00
psi
Atm
Vacuum
Atm
Vacuum
Oven Program
Isothermal
Ramps
Ramp Rate (°C/min)
Temp (°C)
Hold Time (min)
Ramp Rate (°C/min)
Temp (°C)
Hold Time (min)
Number of Ramps (1-4)
40
1
40
0.35
1
8.5
330
1
24
330
0.35
Control Method
Constant Flow
Results
Solve for
Efficiency
Speed
Translate
Custom
Run Time
36.12
12.78
min
Speed
2.83
x
Use Flow Calculator Values
EZGC™ Flow Calculator
Carrier Gas
Helium
Column
Length
30.00
m
Inner Diameter
0.25
mm
Film Thickness
0.25
µm
Temperature
40.00
°C
Control Parameters
Outlet Flow
Optimum Range
1.4 to 2.0 mL/min
1.40
mL/min
Average Velocity
42.74
cm/sec
Holdup Time
1.17
min
Inlet Pressure
psi
11.42
psi
Outlet Pressure (abs)
0.00
psi
Atm
Vacuum
Inlet
Temperature
250.00
°C
Liner Volume
1.00
mL
Flow
1.40
mL/min
Splitless Valve Time
1.1 to 1.5
min
Use MT Original Values
Use MT Translation Values
Download
EZGC™ Method Translator and Flow Calculator
For Windows 8/7/Vista/XP

# GC Column Length Determination

- Using Holdup Time and the Flow Calculator
- Upon initial GC column installation
- Enables accurate Electronic Pneumatic Control of GC carrier gas flow

- Also used after column trimming

# EZGC™ Flow Calculator

## Carrier Gas

Helium

## Column

| | | |
|---|---|---|
| Length | 30.00 | m |
| Inner Diameter | 0.25 | mm |
| Film Thickness | 0.25 | µm |
| Temperature | 90 | °C |

## Control Parameters

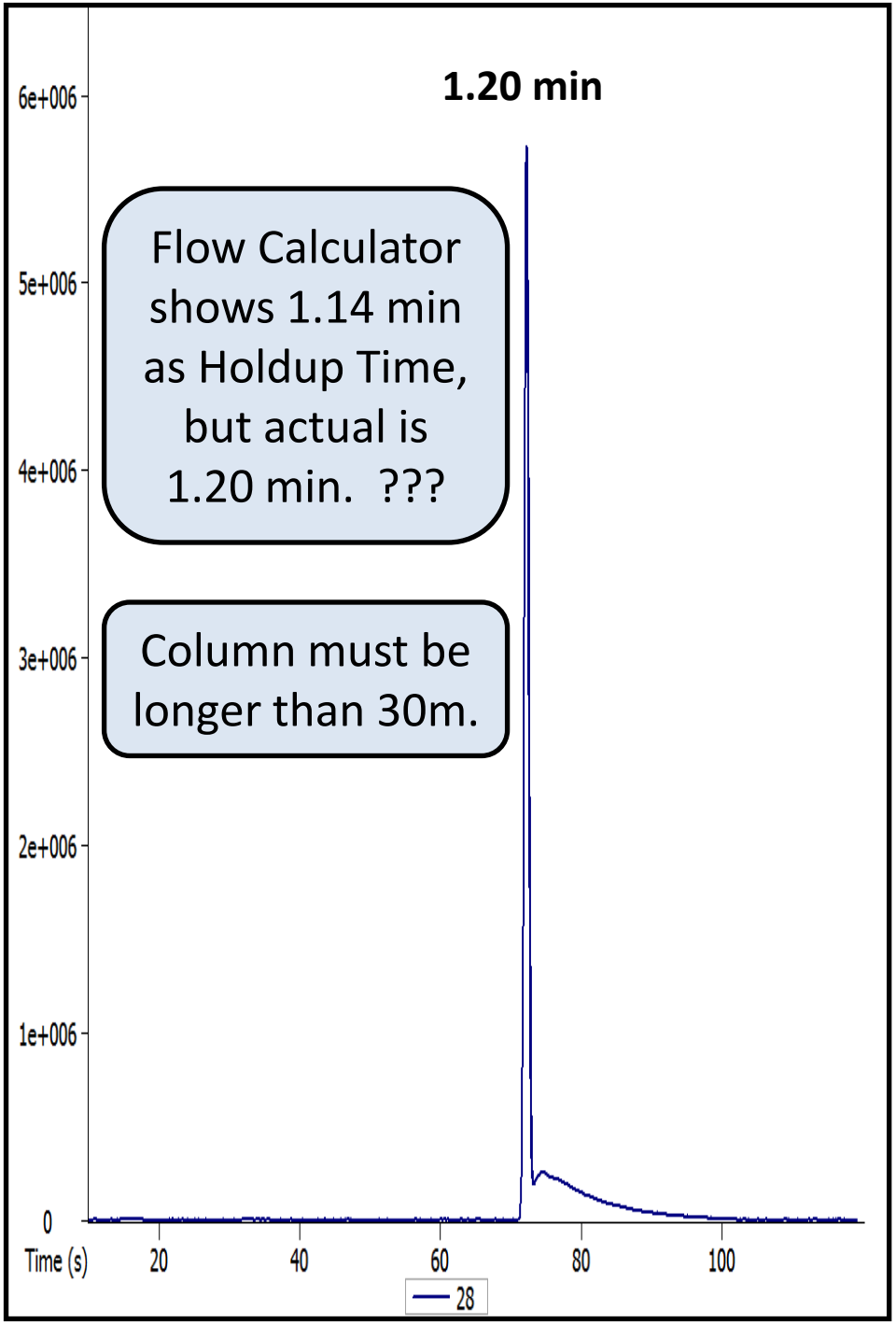
| | | | |
|---|---|---|---|
| Outlet Flow | Optimum Range 1.4 to 2.0 mL/min | 1.40 | mL/min |
| Average Velocity | | 43.73 | cm/sec |
| Holdup Time | | 1.14 | min |
| Inlet Pressure (gauge) | | 14.91 | psi |
| Outlet Pressure (abs) | | 0.00 | psi |

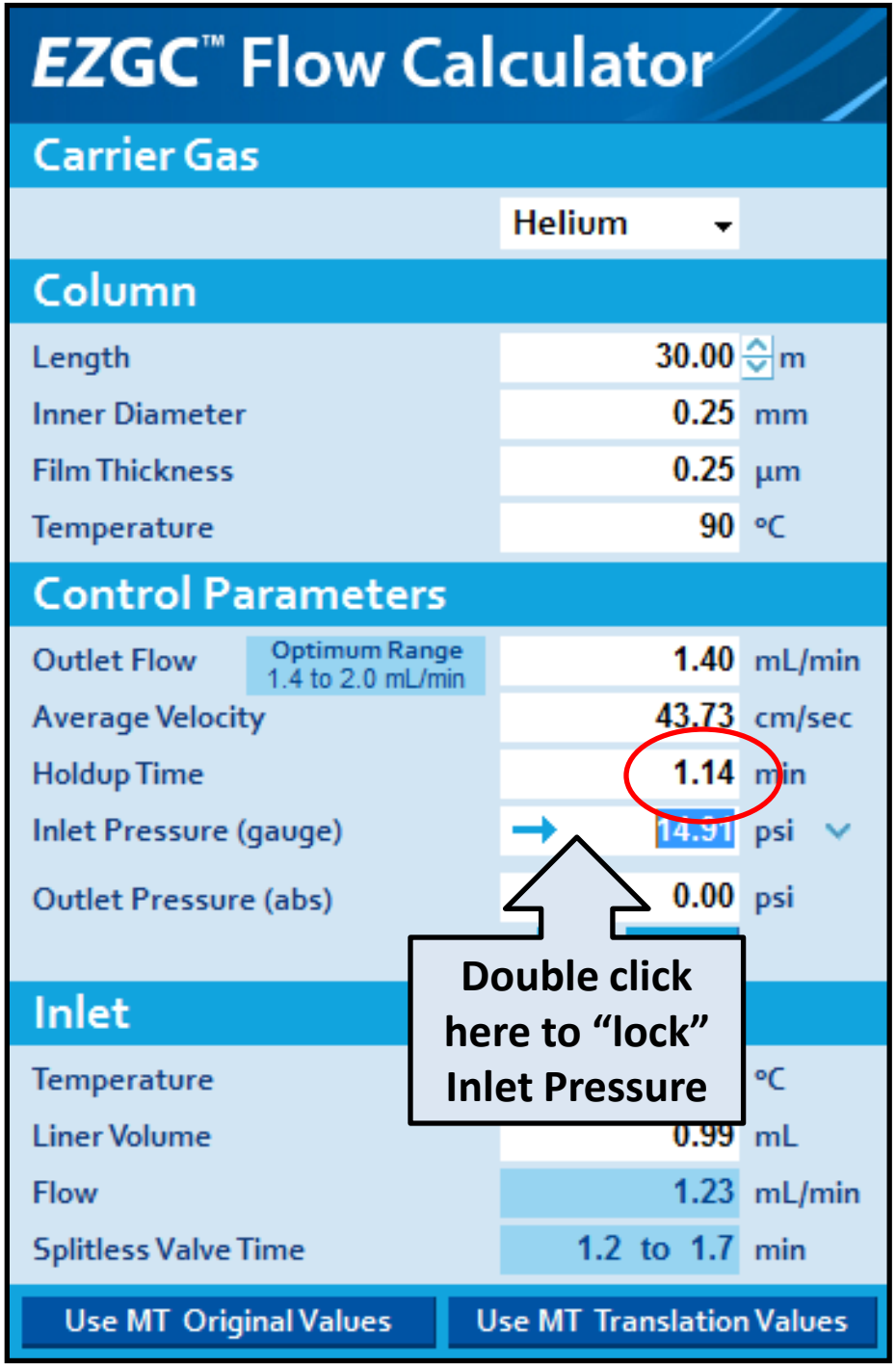
Atm | Vacuum

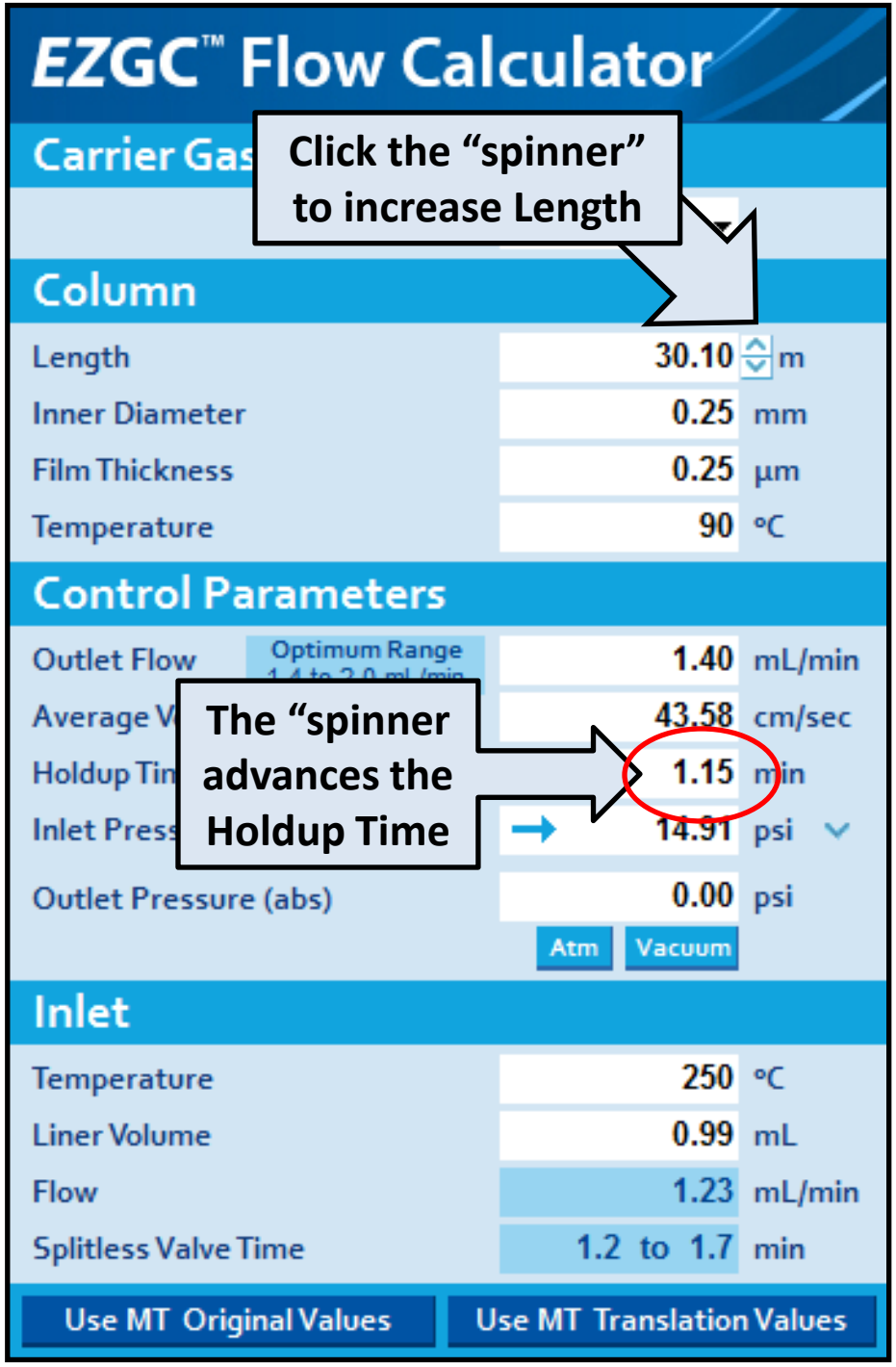
## Inlet

| | | |
|---|---|---|
| Temperature | 250 | °C |
| Liner Volume | 0.99 | mL |
| Flow | 1.23 | mL/min |
| Splitless Valve Time | 1.2 to 1.7 | min |

Use MT Original Values | Use MT Translation Values




EZGC™ Flow Calculator
Carrier Gas
Helium
Column
Length 30.00 m
Inner Diameter 0.25 mm
Film Thickness 0.25 µm
Temperature 90 °C
Control Parameters
Outlet Flow Optimum Range 1.4 to 2.0 mL/min 1.40 mL/min
Average Velocity 43.73 cm/sec
Holdup Time 1.14 min
Inlet Pressure (gauge) 14.91 psi
Outlet Pressure (abs) 0.00 psi
Double click here to "lock" Inlet Pressure
Inlet
Temperature °C
Liner Volume 0.99 mL
Flow 1.23 mL/min
Splitless Valve Time 1.2 to 1.7 min
Use MT Original Values
Use MT Translation Values


EZGC™ Flow Calculator
Carrier Gas
Click the "spinner" to increase Length
Column
Length 30.10 m
Inner Diameter 0.25 mm
Film Thickness 0.25 µm
Temperature 90 °C
Control Parameters
Outlet Flow Optimum Range 1.40 mL/min
Average V 43.58 cm/sec
Holdup Tin 1.15 min
Inlet Press 14.91 psi
The "spinner advances the Holdup Time
Outlet Pressure (abs) 0.00 psi
Atm
Vacuum
Inlet
Temperature 250 °C
Liner Volume 0.99 mL
Flow 1.23 mL/min
Splitless Valve Time 1.2 to 1.7 min
Use MT Original Values
Use MT Translation Values

# EZGC™ Flow Calculator

## Carrier Gas

Helium

## Column

| | | |
|---|---|---|
| Length | 30.70 | m |
| Inner Diameter | 0.25 | mm |
| Film Thickness | 0.25 | µm |
| Temperature | 90 | °C |

## Control Parameters

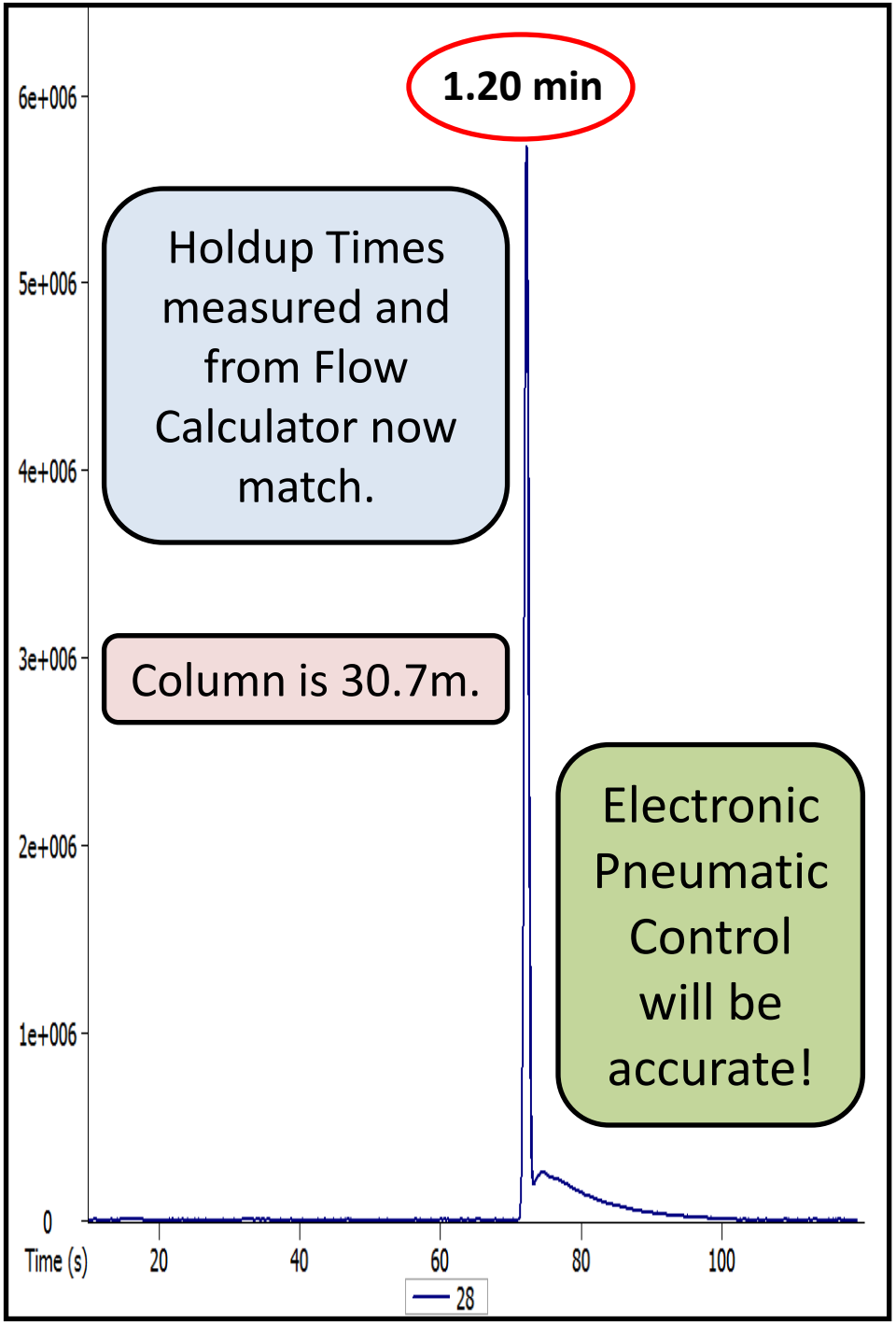
| | | | |
|---|---|---|---|
| Outlet Flow | Optimum Range 1.4 to 2.0 mL/min | 1.37 | mL/min |
| Average Velocity | | 42.74 | cm/sec |
| Holdup Time | | 1.20 | min |
| Inlet Pressure (gauge) | | 14.91 | psi |
| Outlet Pressure (abs) | | 0.00 | psi |

Atm | Vacuum

## Inlet

| | | |
|---|---|---|
| Temperature | 250 | °C |
| Liner Volume | 0.99 | mL |
| Flow | 1.20 | mL/min |
| Splitless Valve Time | 1.2 to 1.7 | min |

Use MT Original Values | Use MT Translation Values



# EZGC™ Flow Calculator

## Carrier Gas

Helium

## Column

| | | |
|---|---|---|
| Length | 30.70 | m |
| Inner Diameter | 0.25 | mm |
| Film Thickness | 0.25 | µm |
| Temperature | 90 | °C |

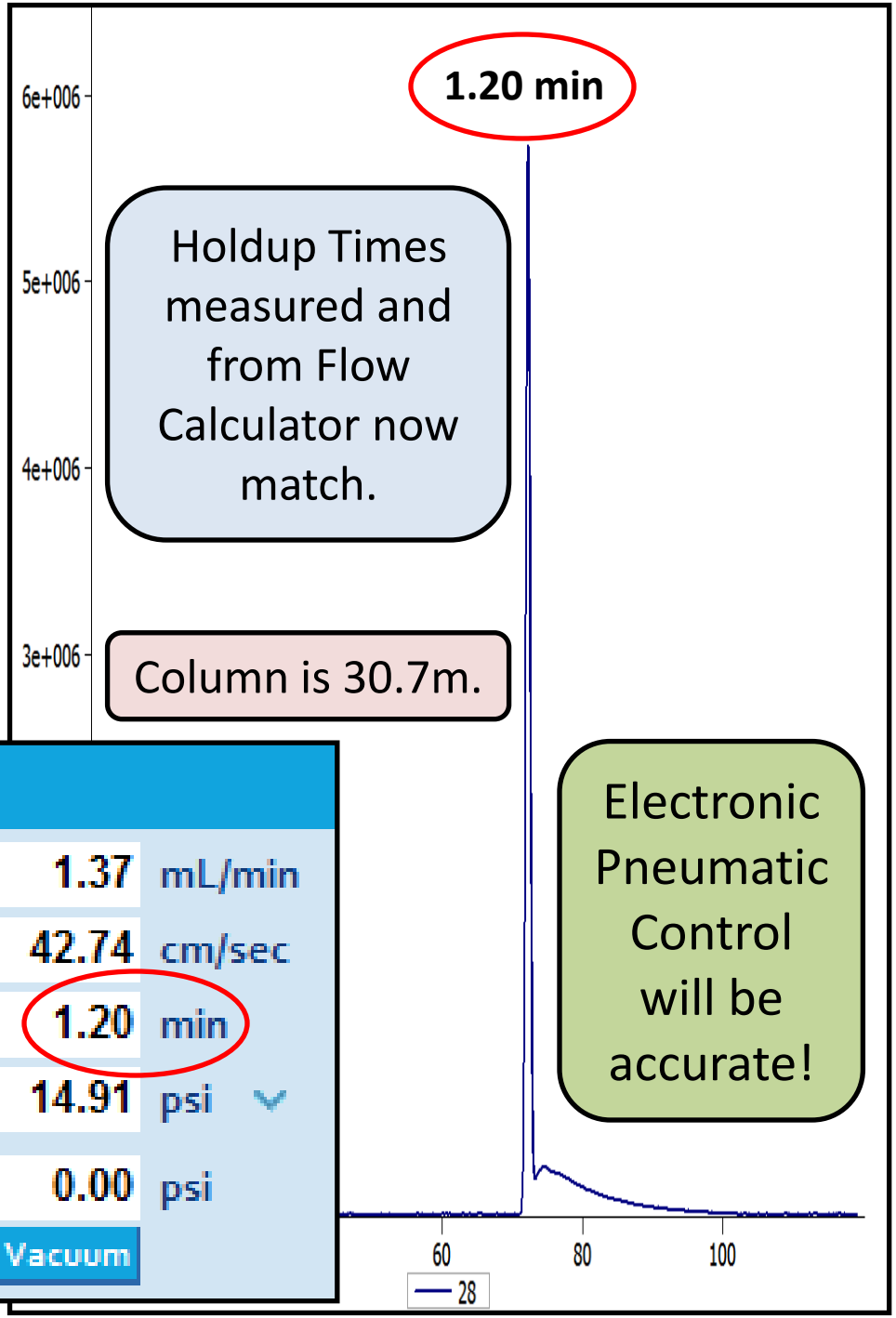
## Control Parameters

| | Optimum Range 1.4 to 2.0 mL/min | | |
|---|---|---|---|
| Outlet Flow | | 1.37 | mL/min |
| Average Velocity | | 42.74 | cm/sec |

## Control Parameters

| | Optimum Range 1.4 to 2.0 mL/min | | |
|---|---|---|---|
| Outlet Flow | | 1.37 | mL/min |
| Average Velocity | | 42.74 | cm/sec |
| Holdup Time | | 1.20 | min |
| Inlet Pressure (gauge) | | 14.91 | psi |
| Outlet Pressure (abs) | | 0.00 | psi |

Atm Vacuum




Holdup Times measured and from Flow Calculator now match.

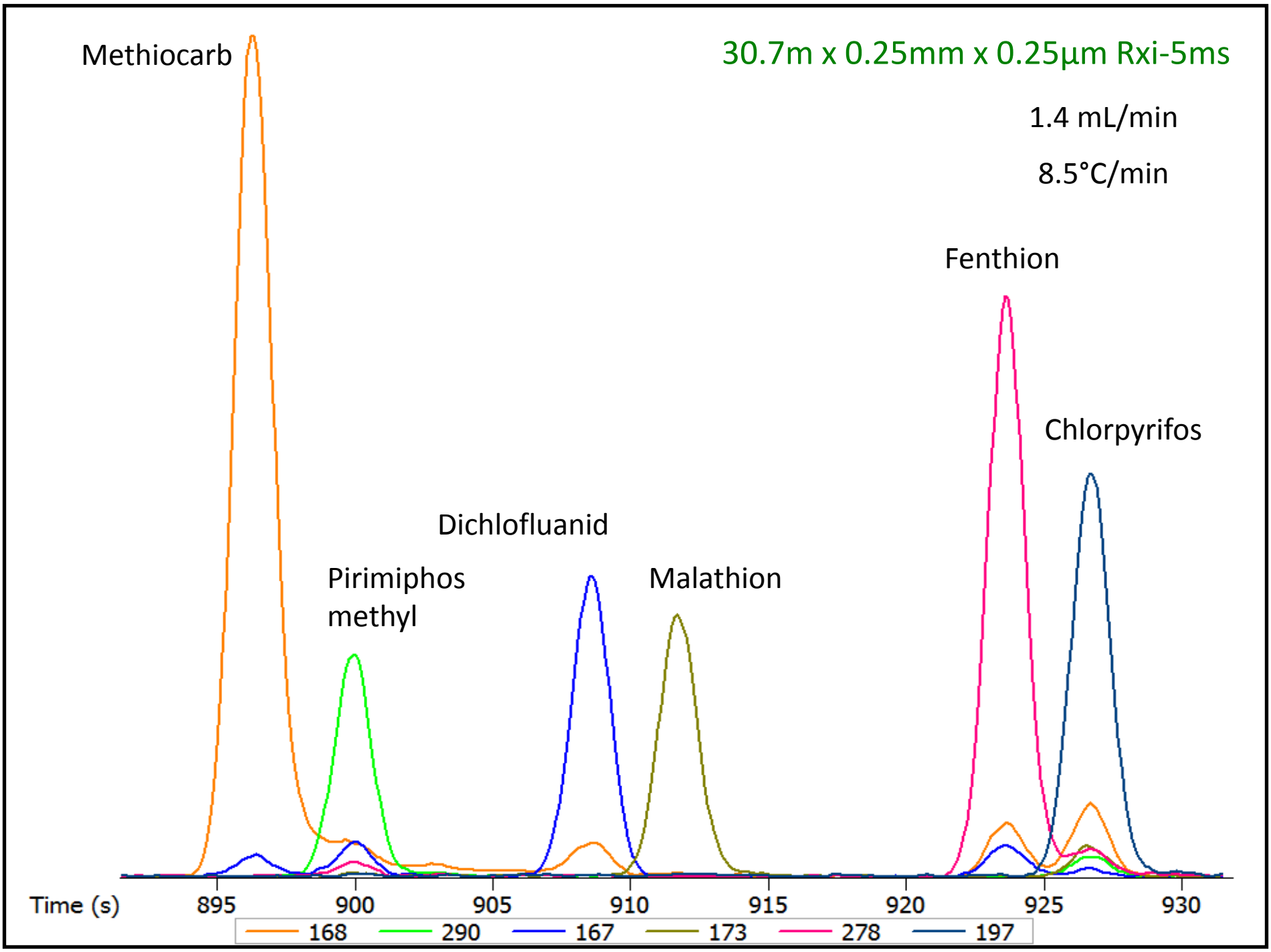
Column is 30.7m.

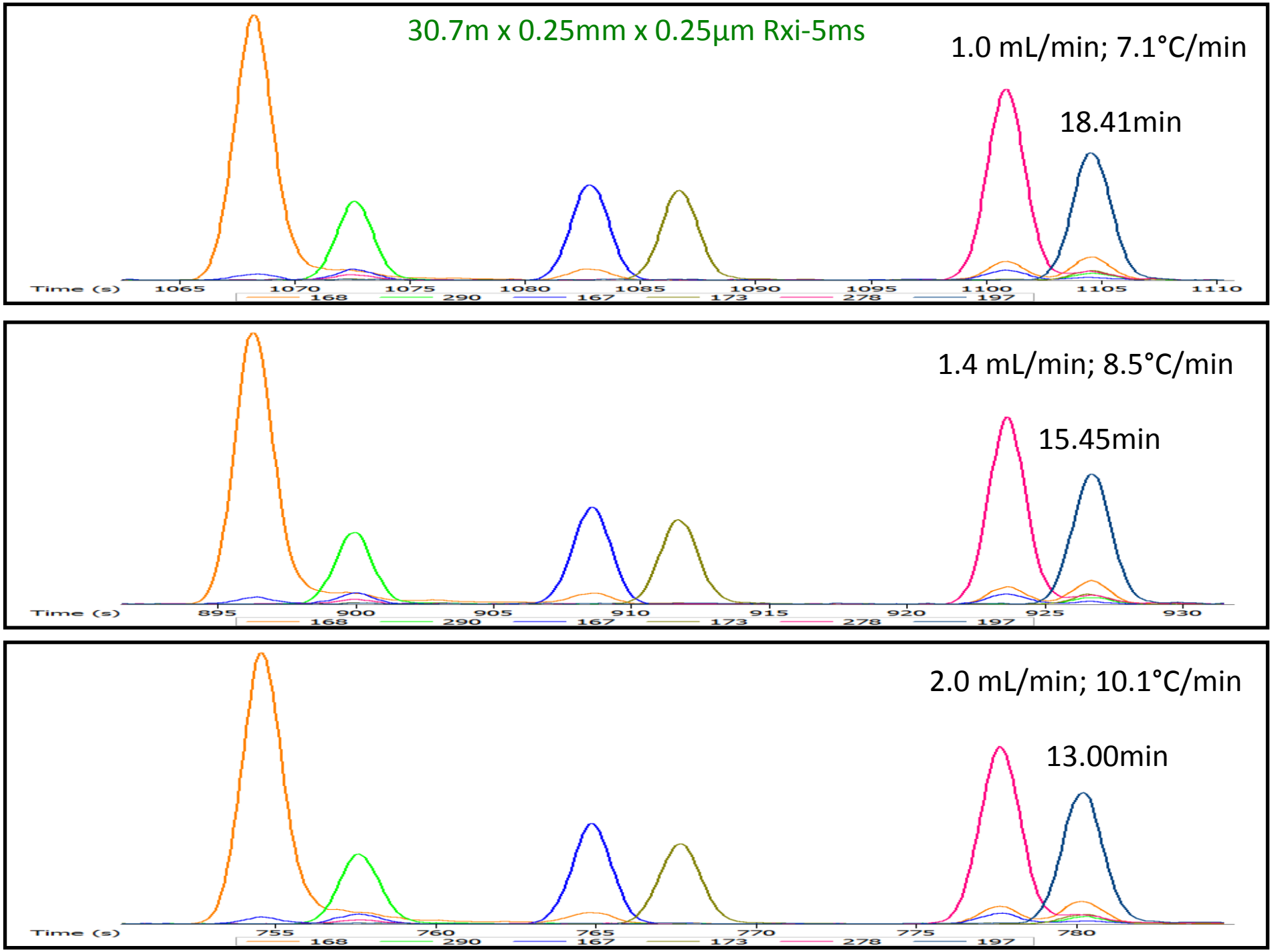
Electronic Pneumatic Control will be accurate!

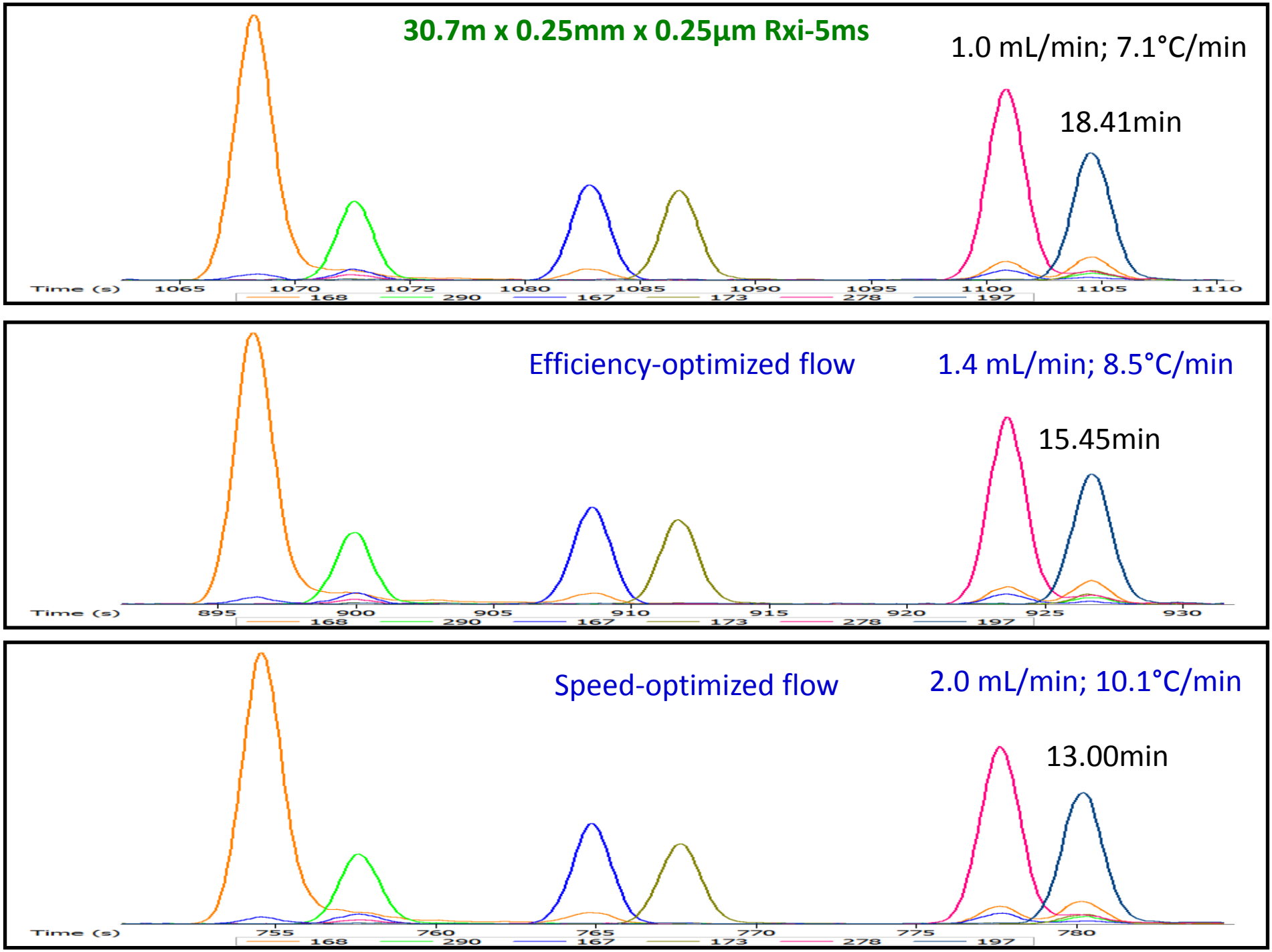
# Combining Optimized Flow and Optimal Heating Rate

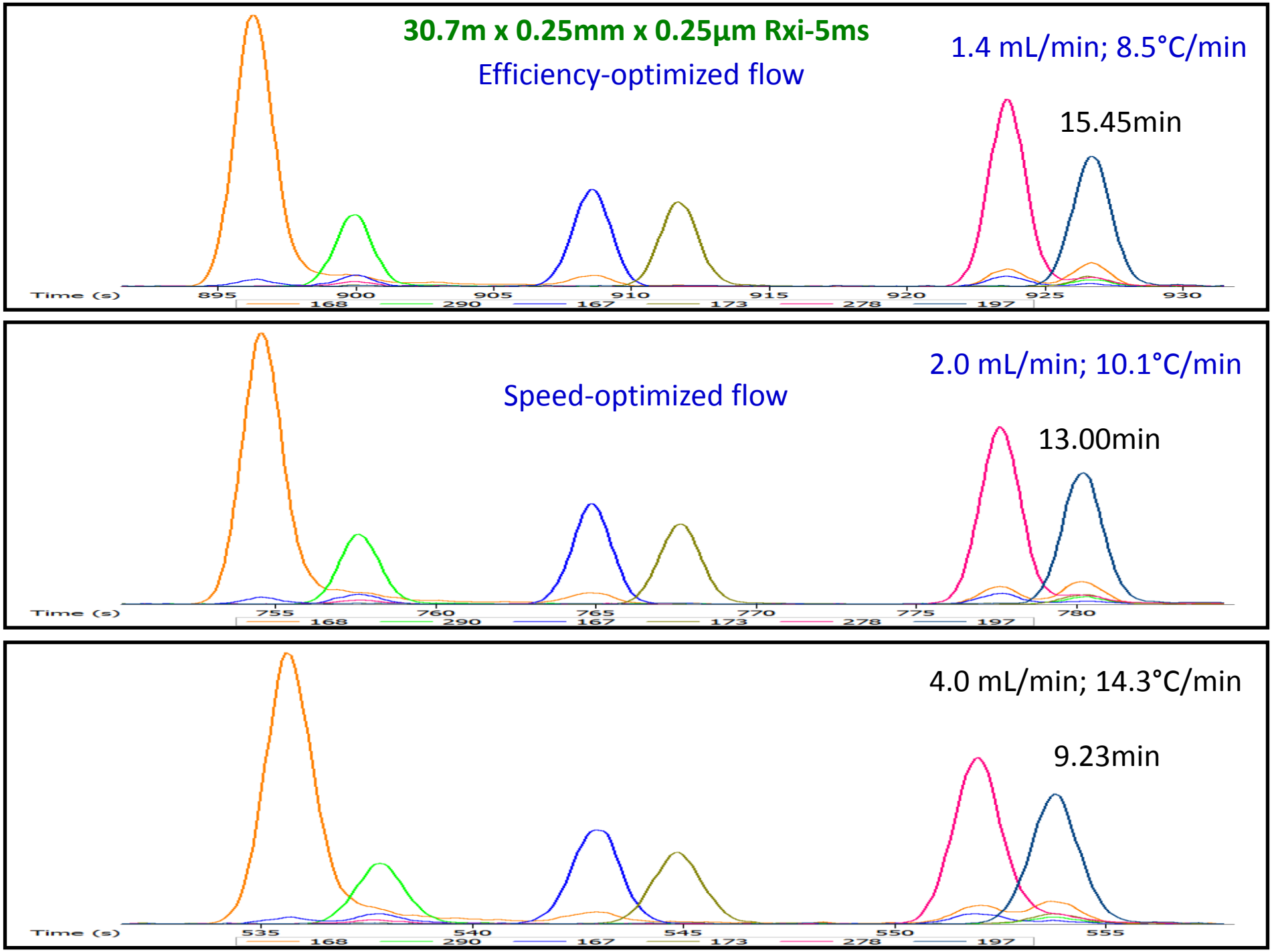
| GC Column | Detector | He EOF mL/min | Avg Vel cm/sec | Holdup time (min) | OHR °C/min | Anal time min |
|---|---|---|---|---|---|---|
| 60m x 0.25mm x 0.25µm | MS | 1.4 | 31 | 3.23 | 3.1 | 74.2 |
| 30m x 0.25mm x 0.25µm | MS | 1.4 | 44 | 1.14 | 8.8 | 26.1 |
| 15m x 0.25mm x 0.25µm | MS | 1.4 | 62 | 0.40 | 25.0 | 9.2 |
| | | | | | | |
| 20m x 0.18mm x 0.18µm | MS | 1.0 | 39 | 0.74 | 13.5 | 17.0 |
| | | | | | | |
| 60m x 0.25mm x 0.25µm | ECD | 1.4 | 27 | 3.71 | 2.7 | 85.1 |
| 30m x 0.25mm x 0.25µm | ECD | 1.4 | 35 | 1.45 | 6.9 | 33.3 |
| 15m x 0.25mm x 0.25µm | ECD | 1.4 | 42 | 0.60 | 16.7 | 13.8 |

Mass spectrometer is a vacuum-outlet detector.
Holdup time is at 90°C.
Analysis time is based on 90 to 320°C oven program.


Methiocarb
30.7m x 0.25mm x 0.25µm Rxi-5ms
1.4 mL/min
8.5°C/min
Fenthion
Chlorpyrifos
Dichlofluanid
Pirimiphos methyl
Malathion
Time (s)
895
900
905
910
915
920
925
930
168
290
167
173
278
197


30.7m x 0.25mm x 0.25µm Rxi-5ms
1.0 mL/min; 7.1°C/min
18.41min
Time (s)
1065
1070
1075
1080
1085
1090
1095
1100
1105
1110
168
290
167
173
278
197
1.4 mL/min; 8.5°C/min
15.45min
Time (s)
895
900
905
910
915
920
925
930
168
290
167
173
278
197
2.0 mL/min; 10.1°C/min
13.00min
Time (s)
755
760
765
770
775
780
168
290
167
173
278
197


30.7m x 0.25mm x 0.25µm Rxi-5ms
1.0 mL/min; 7.1°C/min
18.41min
Time (s)
1065 1070 1075 1080 1085 1090 1095 1100 1105 1110
168 290 167 173 278 197
Efficiency-optimized flow
1.4 mL/min; 8.5°C/min
15.45min
Time (s)
895 900 905 910 915 920 925 930
168 290 167 173 278 197
Speed-optimized flow
2.0 mL/min; 10.1°C/min
13.00min
Time (s)
755 760 765 770 775 780
168 290 167 173 278 197


30.7m x 0.25mm x 0.25µm Rxi-5ms
Efficiency-optimized flow
1.4 mL/min; 8.5°C/min
15.45min
Time (s)
895 900 905 910 915 920 925 930
168 290 167 173 278 197
Speed-optimized flow
2.0 mL/min; 10.1°C/min
13.00min
Time (s)
755 760 765 770 775 780
168 290 167 173 278 197
4.0 mL/min; 14.3°C/min
9.23min
Time (s)
535 540 545 550 555
168 290 167 173 278 197

# We need to know…

Flow rate ✓

Oven program ✓

Accurate column length ✓

Initial oven temperature

Splitless hold time

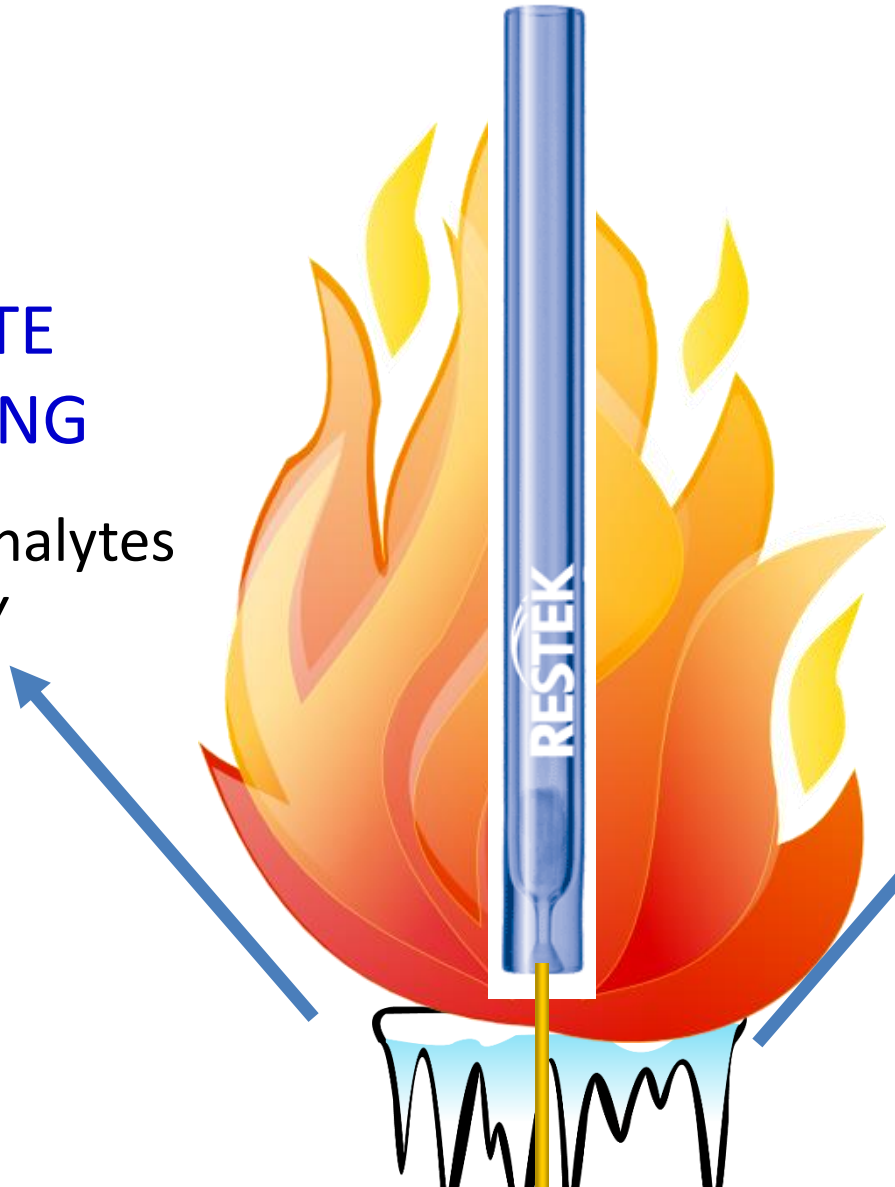
# Initial Oven Temperature

ANALYTE FOCUSING

Cold trap analytes ONLY

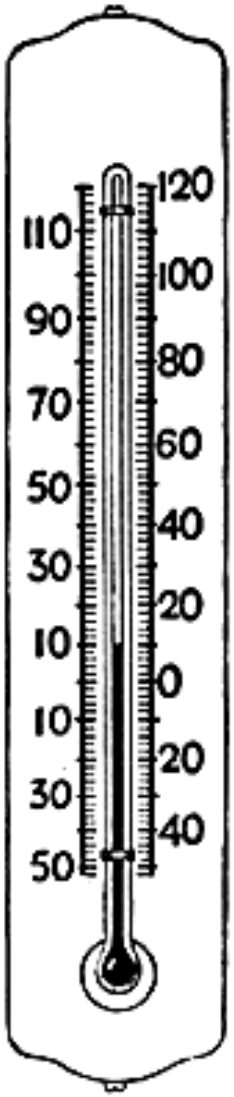
SOLVENT FOCUSING

Cold trap analytes AND solvent



# Initial Oven Temperature

## SOLVENT FOCUSING




Boiling point of 1st analyte

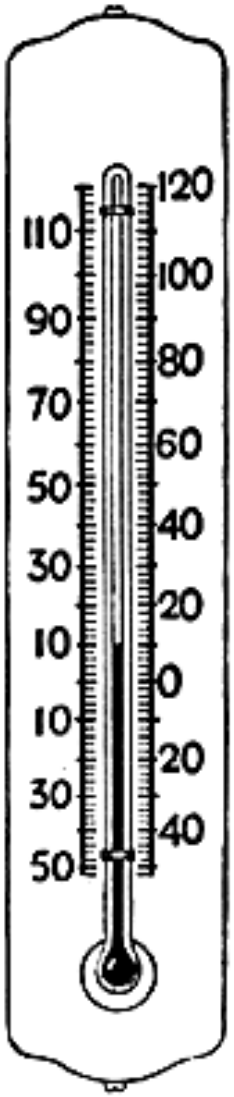
Boiling point of solvent

**20-40°C lower**

Initial Oven Temperature

# Initial Oven Temperature

## ANALYTE FOCUSING




Boiling point of 1st analyte

**20°C lower**

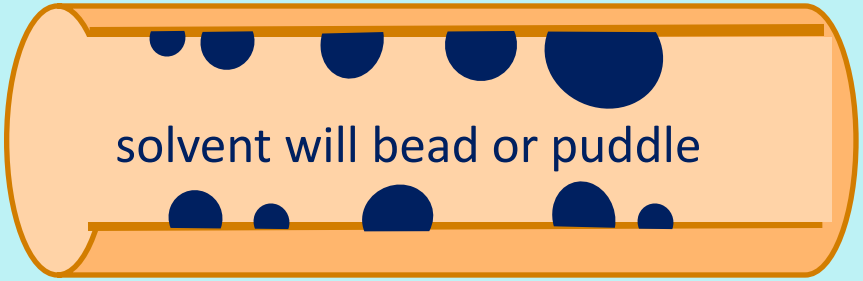
**60-80°C**

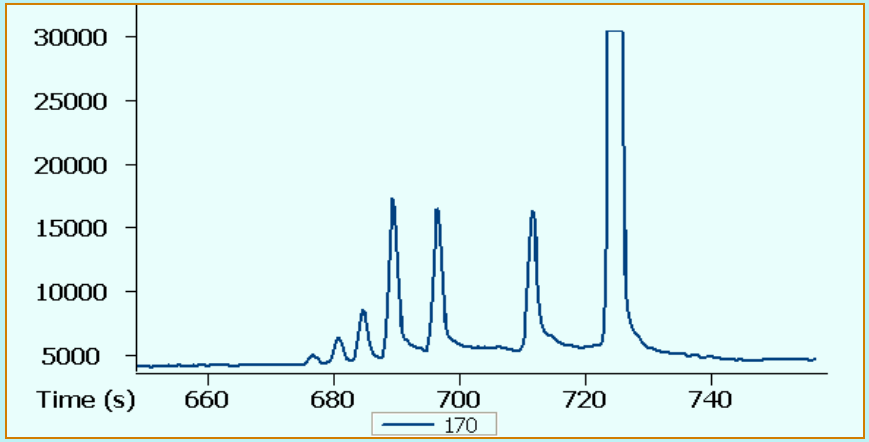
**20°C higher**

Boiling point of solvent

# Solvent Focusing: Solvent Polarity Mismatch

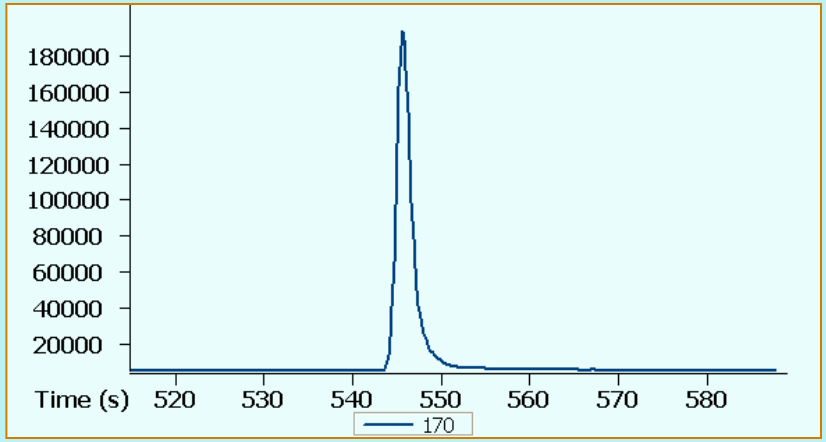
## Mismatched Polarity




o-Phenylphenol

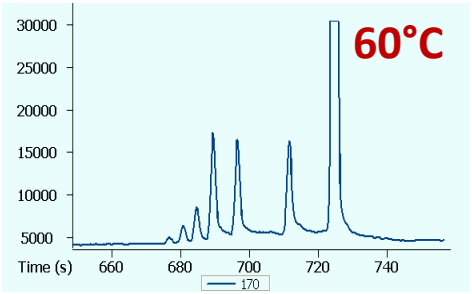
## Polarity Match

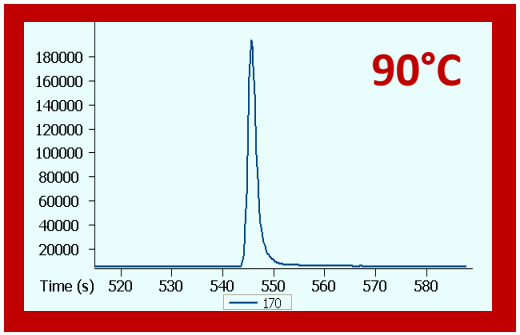



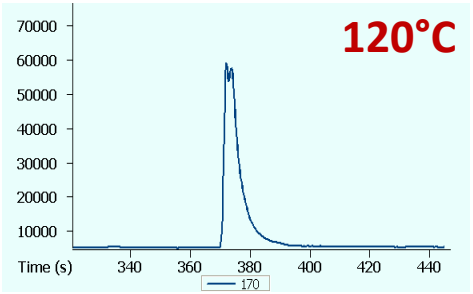

o-Phenylphenol

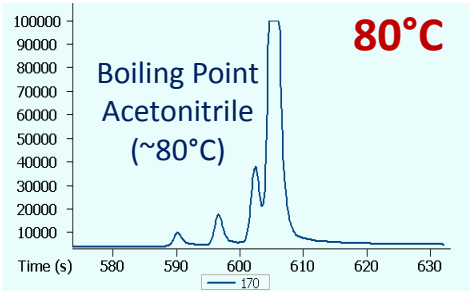
**If solvent boiling point is NOT below that of lowest analyte boiling point focusing of both solvent and analytes**

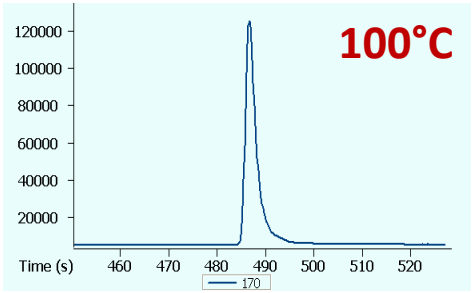
# Initial Oven Temperature

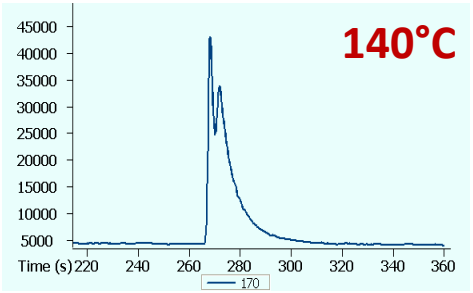



**<u>Solvent Focused:</u>**
**Acetonitrile enters column as liquid and beads because of solvent/stationary phase mismatch**

**<u>Analyte Focused:</u>**
**Acetonitrile is flash vaporized and not cold trapped (condenses) on the front of the column**

**<u>No Cold Trapping</u>**
**Both the acetonitrile and analyte (o-Phenylphenol) are NOT cold trapped effectively on the front of the column**

**o-Phenylphenol, XIC at m/z 170**

# We need to know…

Flow rate ✓

Oven program ✓

Accurate column length ✓

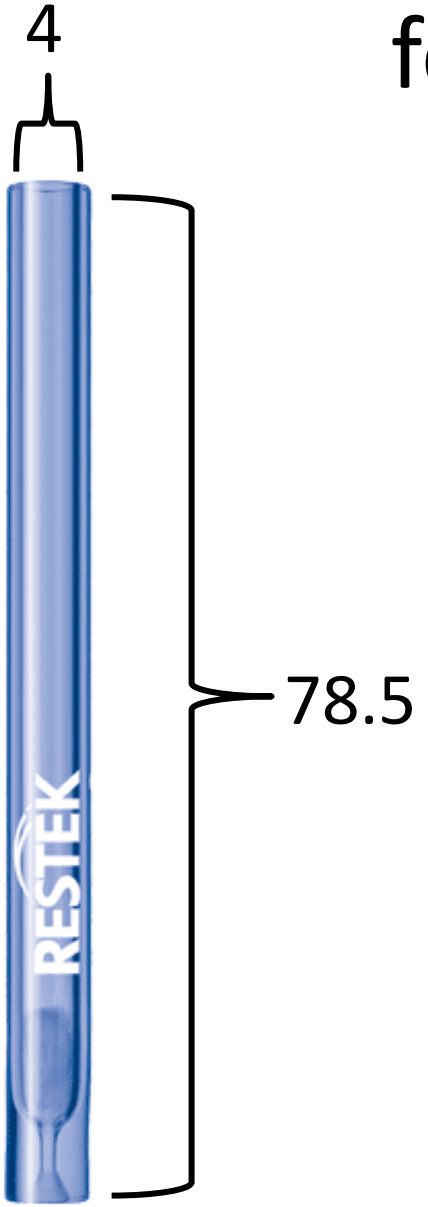
Initial oven temperature ✓

Splitless hold time

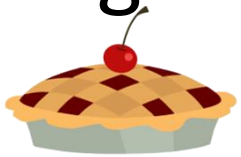
# Splitless Valve Time

Calculating the Splitless Valve Time with the Flow Calculator

# Calculating the GC Inlet Liner Volume for Splitless Valve Time




- Volume of a cylinder
  - $V = \pi r^2 h$
- Inlet liner for Agilent GC
  - 3.1416 (π)



  - 4 mm diameter, 2 mm radius (r)
  - 78.5 mm height (h)
- Liner V = 986 µL (0.99 mL)
  - Ignore wool and taper

# Calculating the GC Inlet Liner Volume for Splitless Valve Time


Liner volume 0.99 mL

Want 1.5 to 2x sweep…

**Inlet**

| | | |
|---|---|---|
| Temperature | 250 | °C |
| Liner Volume | 0.99 | mL |
| Flow | 1.22 | mL/min |
| Splitless Valve Time | 1.2 to 1.7 | min |

Use MT Original Values | Use MT Translation Values

EZGC™ Flow Calculator Splitless Valve Time range is 1.2 to 1.7 min.

**EZGC™ Flow Calculator**

**Carrier Gas**

Helium

**Column**

| | | |
|---|---|---|
| Length | 30.70 | m |
| Inner Diameter | 0.25 | mm |
| Film Thickness | 0.25 | µm |
| Temperature | 90 | °C |

**Control Parameters**

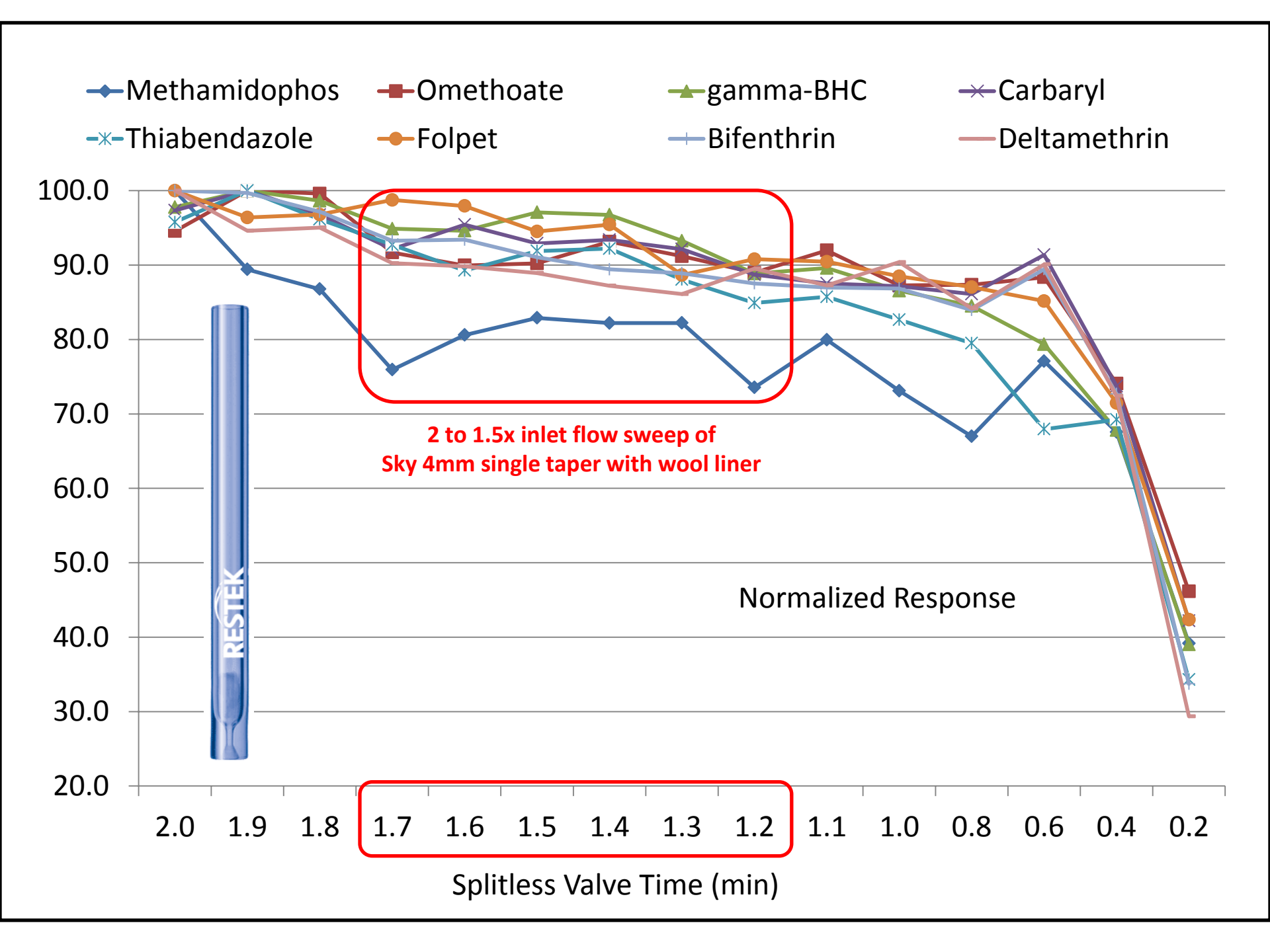
| | | | |
|---|---|---|---|
| Outlet Flow | Optimum Range 1.4 to 2.0 mL/min | 1.40 | mL/min |
| Average Velocity | | 43.23 | cm/sec |
| Holdup Time | | 1.18 | min |
| Inlet Pressure (gauge) | | 15.25 | PSI |
| Outlet Pressure (abs) | | 0.00 | PSI |

Atm | Vacuum

**Inlet**

| | | |
|---|---|---|
| Temperature | 250 | °C |
| Liner Volume | 0.99 | mL |
| Flow | 1.22 | mL/min |
| Splitless Valve Time | 1.2 to 1.7 | min |

Use MT Original Values | Use MT Translation Values


Methamidophos
Omethoate
gamma-BHC
Carbaryl
Thiabendazole
Folpet
Bifenthrin
Deltamethrin
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
2 to 1.5x inlet flow sweep of
Sky 4mm single taper with wool liner
RESTEK
Normalized Response
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.8
0.6
0.4
0.2
Splitless Valve Time (min)

# We need to know…

Flow rate ✓

Oven program ✓

Accurate column length ✓

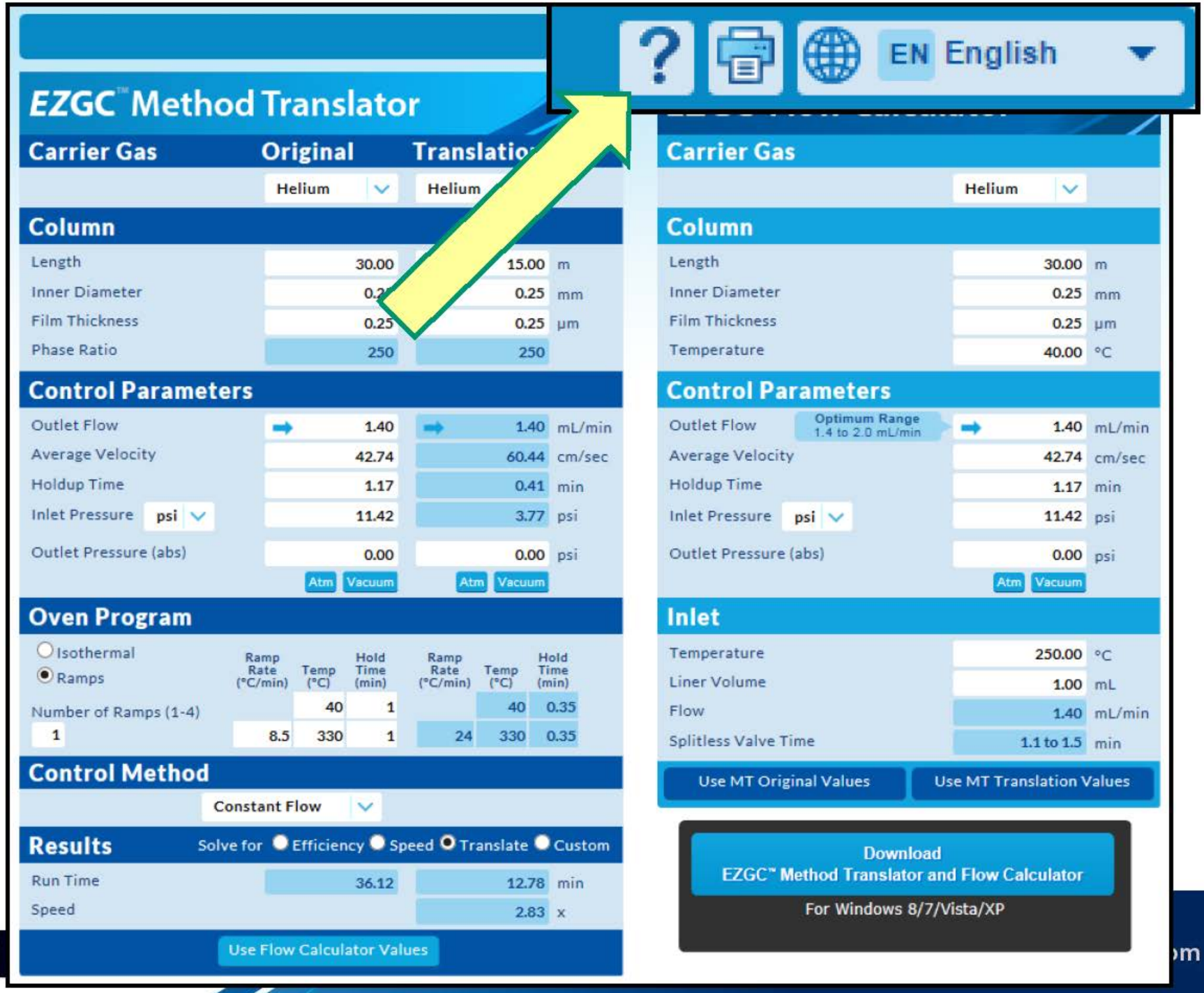
Initial oven temperature ✓

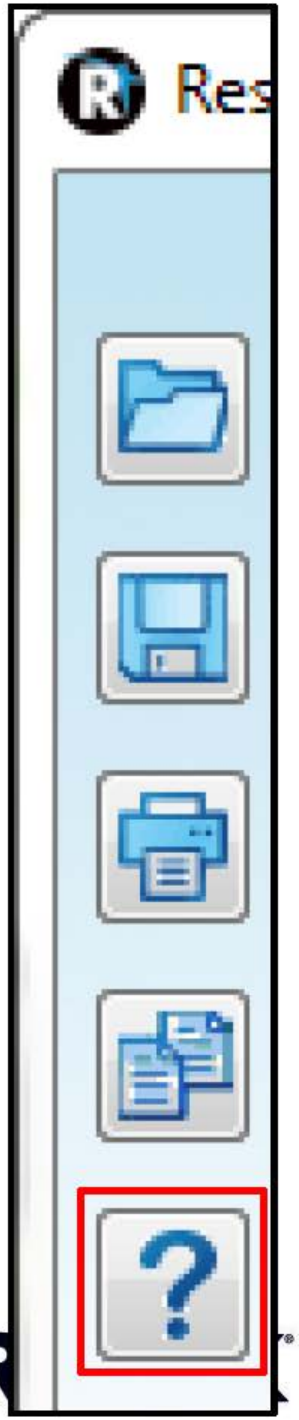
Splitless hold time ✓

# *EZ*GC™ Method Translator / Flow Calculator

*Make our methods better, faster, cheaper!*

- Increasing speed of analysis
  - Decreasing column L and/or ID
  - Switching to a faster carrier gas (e.g., He to $H_2$)
- Updating oven temperature program after column trimming for maintenance
- Improving Original methods in separation and/or speed of analysis
- Translating methods from GC-FID (or other atmospheric outlet detector) to GC-MS (vacuum outlet) or vice versa


EZGC™ Method Translator
EN English
Carrier Gas
Original
Translation
Helium
Helium
Column
Length
30.00
15.00
m
Inner Diameter
0.25
mm
Film Thickness
0.25
0.25
µm
Phase Ratio
250
250
Control Parameters
Outlet Flow
1.40
1.40
mL/min
Average Velocity
42.74
60.44
cm/sec
Holdup Time
1.17
0.41
min
Inlet Pressure
psi
11.42
3.77
psi
Outlet Pressure (abs)
0.00
0.00
psi
Atm
Vacuum
Atm
Vacuum
Oven Program
Isothermal
Ramps
Ramp Rate (°C/min)
Temp (°C)
Hold Time (min)
Ramp Rate (°C/min)
Temp (°C)
Hold Time (min)
Number of Ramps (1-4)
40
1
40
0.35
1
8.5
330
1
24
330
0.35
Control Method
Constant Flow
Results
Solve for
Efficiency
Speed
Translate
Custom
Run Time
36.12
12.78
min
Speed
2.83
x
Use Flow Calculator Values
Carrier Gas
Helium
Column
Length
30.00
m
Inner Diameter
0.25
mm
Film Thickness
0.25
µm
Temperature
40.00
°C
Control Parameters
Outlet Flow
Optimum Range
1.4 to 2.0 mL/min
1.40
mL/min
Average Velocity
42.74
cm/sec
Holdup Time
1.17
min
Inlet Pressure
psi
11.42
psi
Outlet Pressure (abs)
0.00
psi
Atm
Vacuum
Inlet
Temperature
250.00
°C
Liner Volume
1.00
mL
Flow
1.40
mL/min
Splitless Valve Time
1.1 to 1.5
min
Use MT Original Values
Use MT Translation Values
Download
EZGC™ Method Translator and Flow Calculator
For Windows 8/7/Vista/XP



Glossary

# *EZ*GC™ Method Translator and Flow Calculator Glossary

The *EZ*GC™ Method Translator is a tool built for gas chromatography (GC) method development. Generally, the goal of Method Translation is to allow alteration of GC column format, carrier gas, flow, etc., while keeping peak elution order—NOT retention times—the same. (Note that Method Translation assumes that the GC stationary phase type remains the same between Original and Translation methods.)

Some of the most practical uses for Restek's *EZ*GC™ Method Translator are listed below:

- Increasing speed of analysis through decreasing column length and/or decreasing inner diameter and/or switching to a faster carrier gas (e.g., going from helium to hydrogen).
- Updating the oven temperature program through Translation after column trimming for maintenance so peak elution orders do not change.
- Improving Original methods in separation and/or speed of analysis by solving for Efficiency or Speed in Translation.
- Translating methods from GC-FID (or other atmospheric outlet detector) to GC-MS (vacuum outlet) or vice versa.

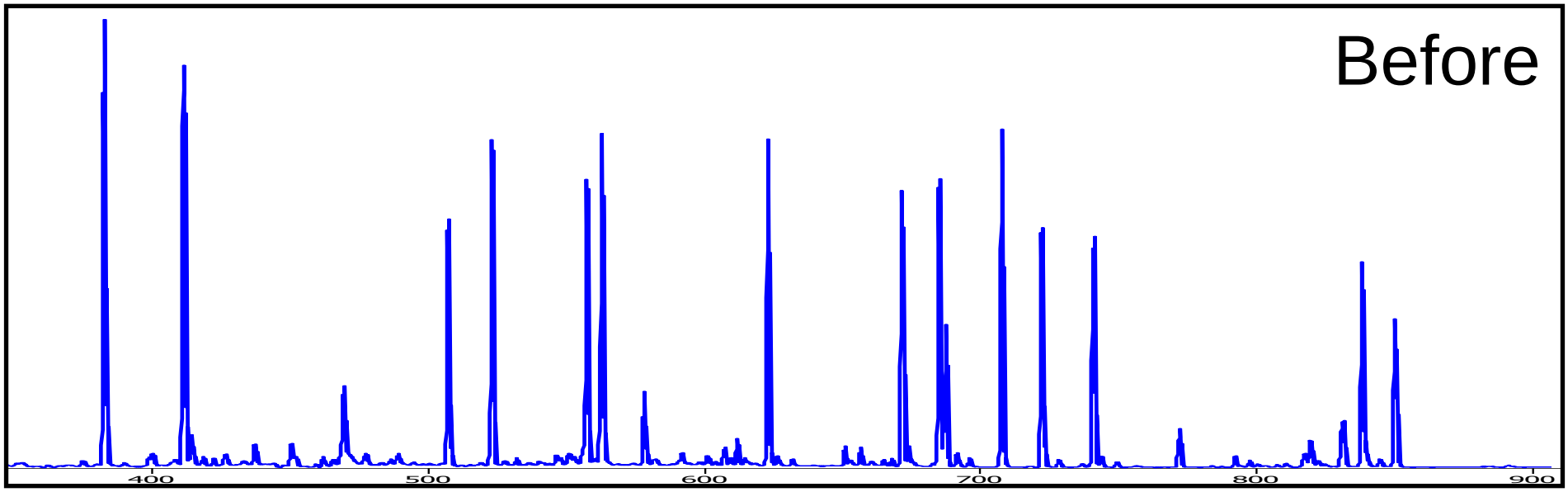
## Basic Navigation in the *EZ*GC™ Method Translator and Flow Calculator

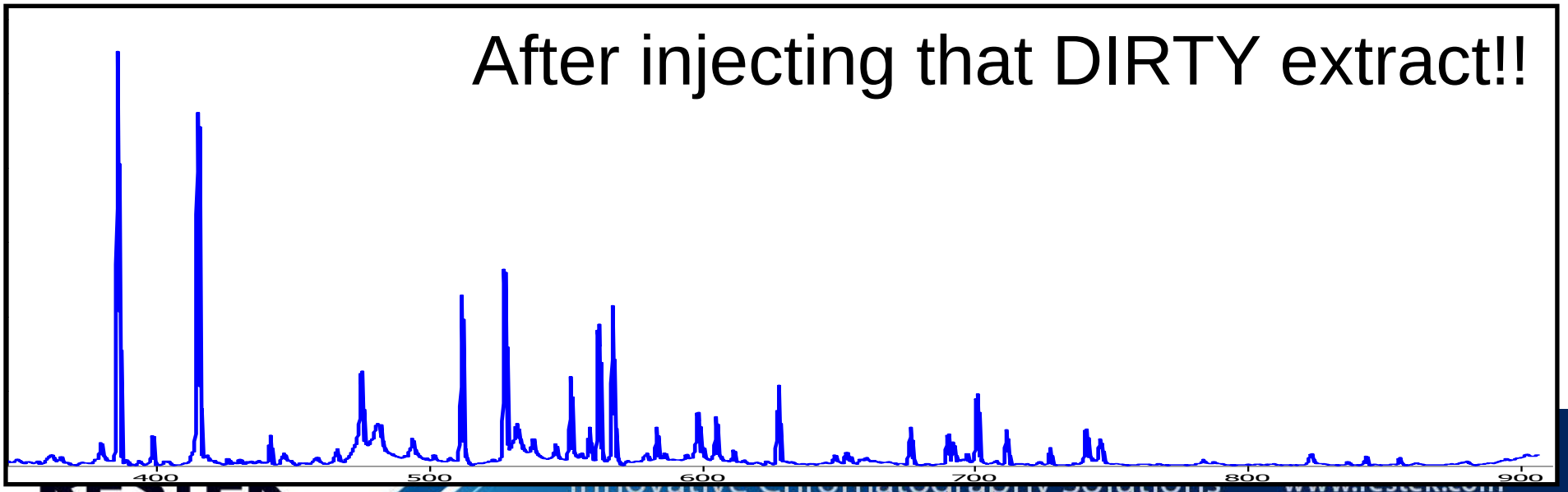
"White" cells are user-entry cells. "Blue" cells are locked cells that contain calculated values. In the Method Translator, the Translation's Control Parameters can be unlocked by selecting the Custom translation method in the Results section.

Highlighting numerical values using the mouse allows easy user entry of new values. A double mouse click in any user-entry cell highlights the value automatically for user entry. Hitting the Tab key while in a cell updates the cell with the user entered value and moves to the next cell for additional user entry, if necessary.

In the Control Parameters section for both the Method Translator and Flow Calculator, a double mouse click in the Outlet Flow, Average Velocity, Holdup Time, or Inlet Pressure cell will make that cell the "set point" around which the other control parameters are calculated. Column dimensions (and Temperature, in the Flow Calculator) can then be changed, and the set point value will remain fixed. A blue arrow denotes the "set point" cell.

# Column Trimming for Maintenance



# No Method Translation

- Trimming column for maintenance
- But, not updating column length for flow control
- And, updating column length, but not translating oven temperature program

I just want to trim my column and change NOTHING!

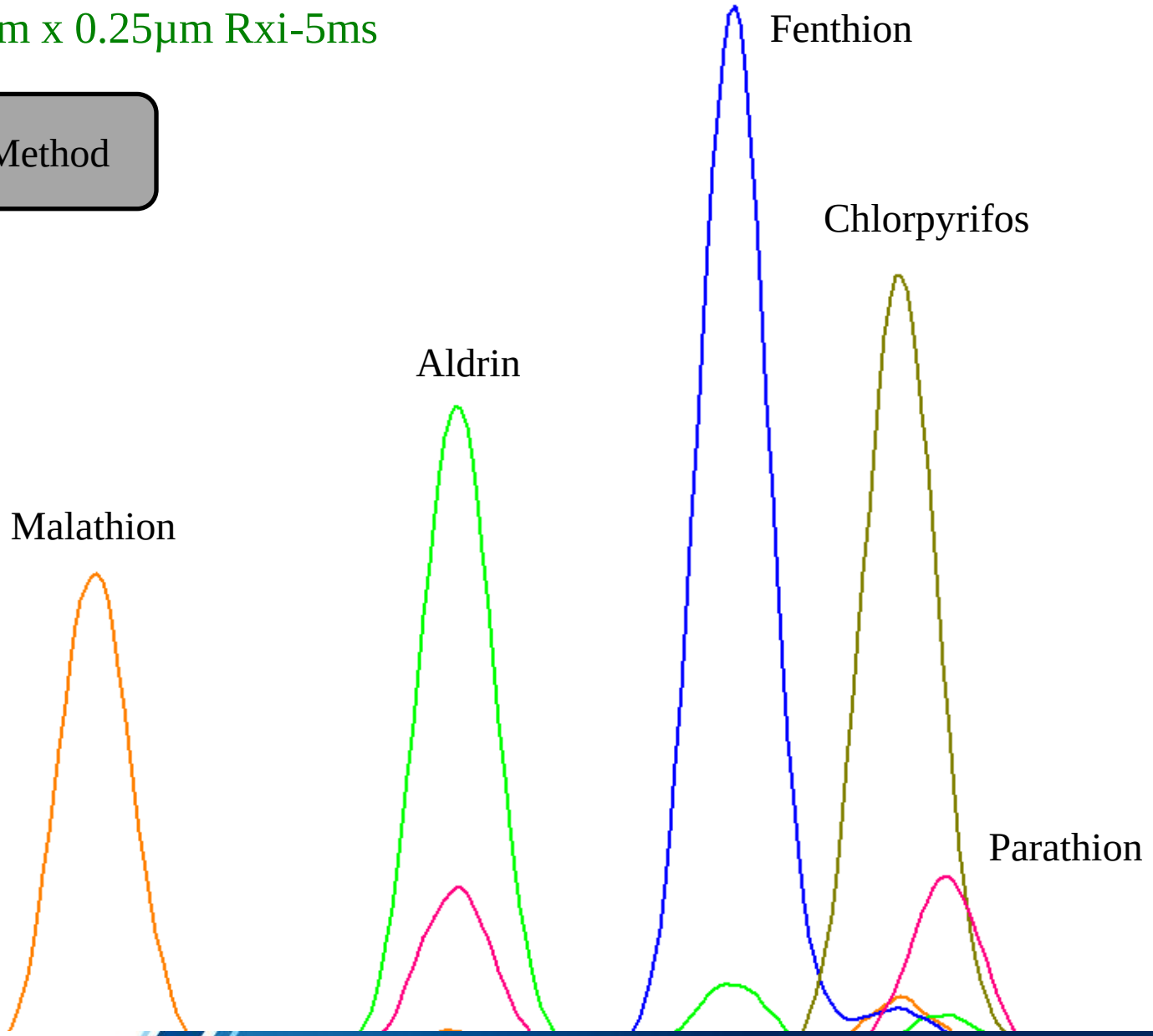
# What if you don't translate?

I just want to trim my column and change NOTHING!

I will input my new column length but NOT my oven program rate!

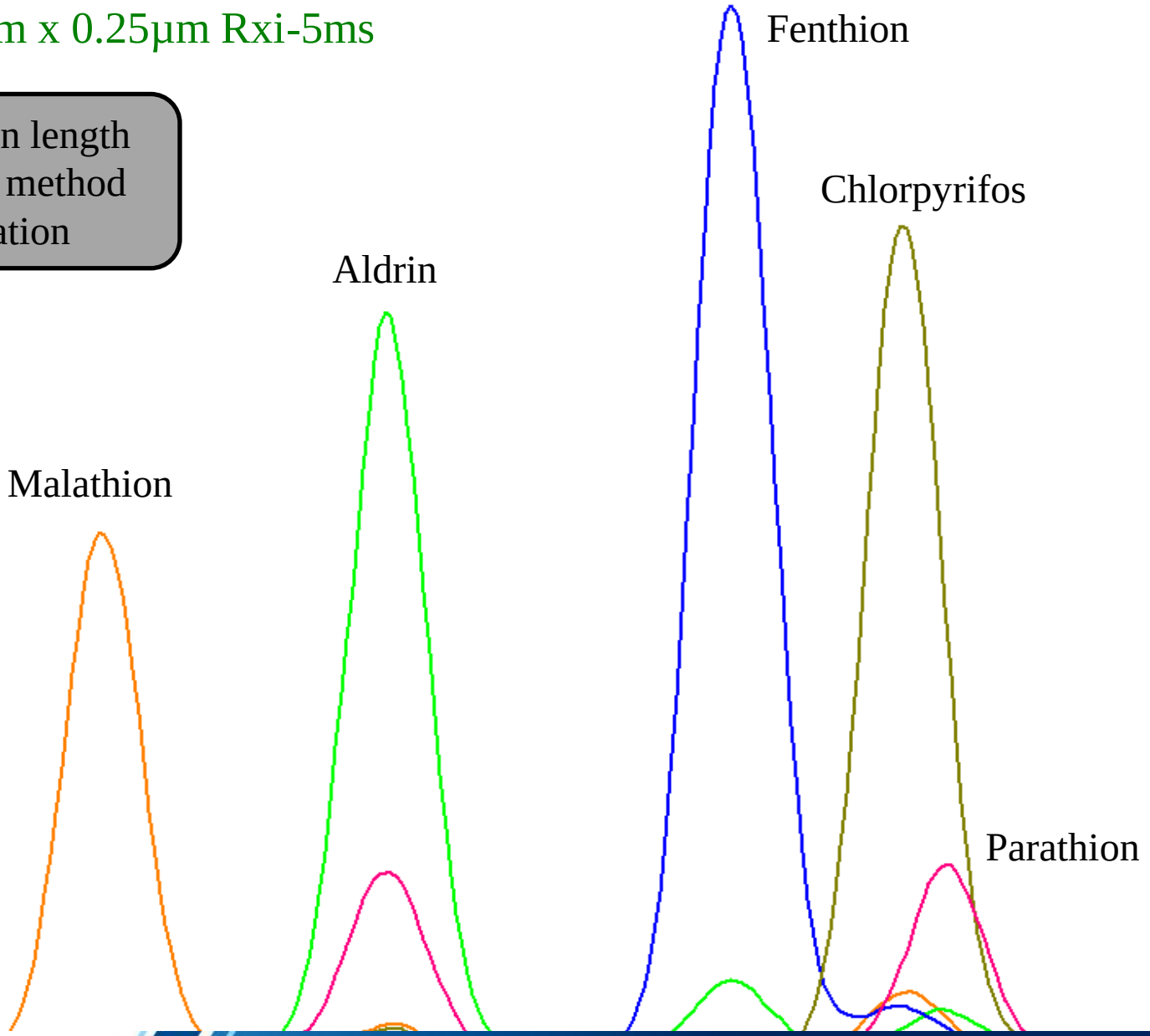
30.7m x 0.25mm x 0.25µm Rxi-5ms

Original Method



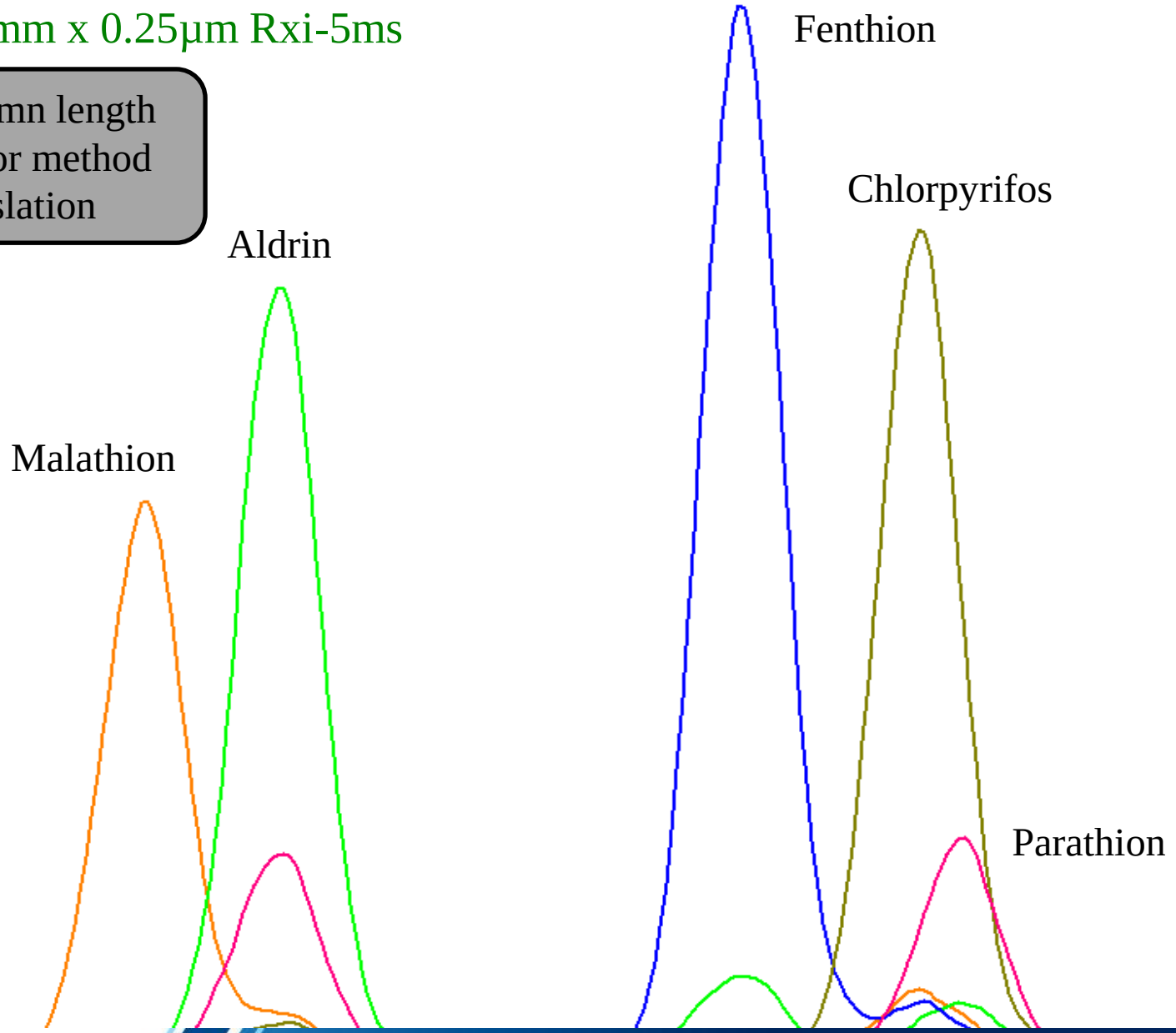
29.6m x 0.25mm x 0.25µm Rxi-5ms

No column length update or method translation



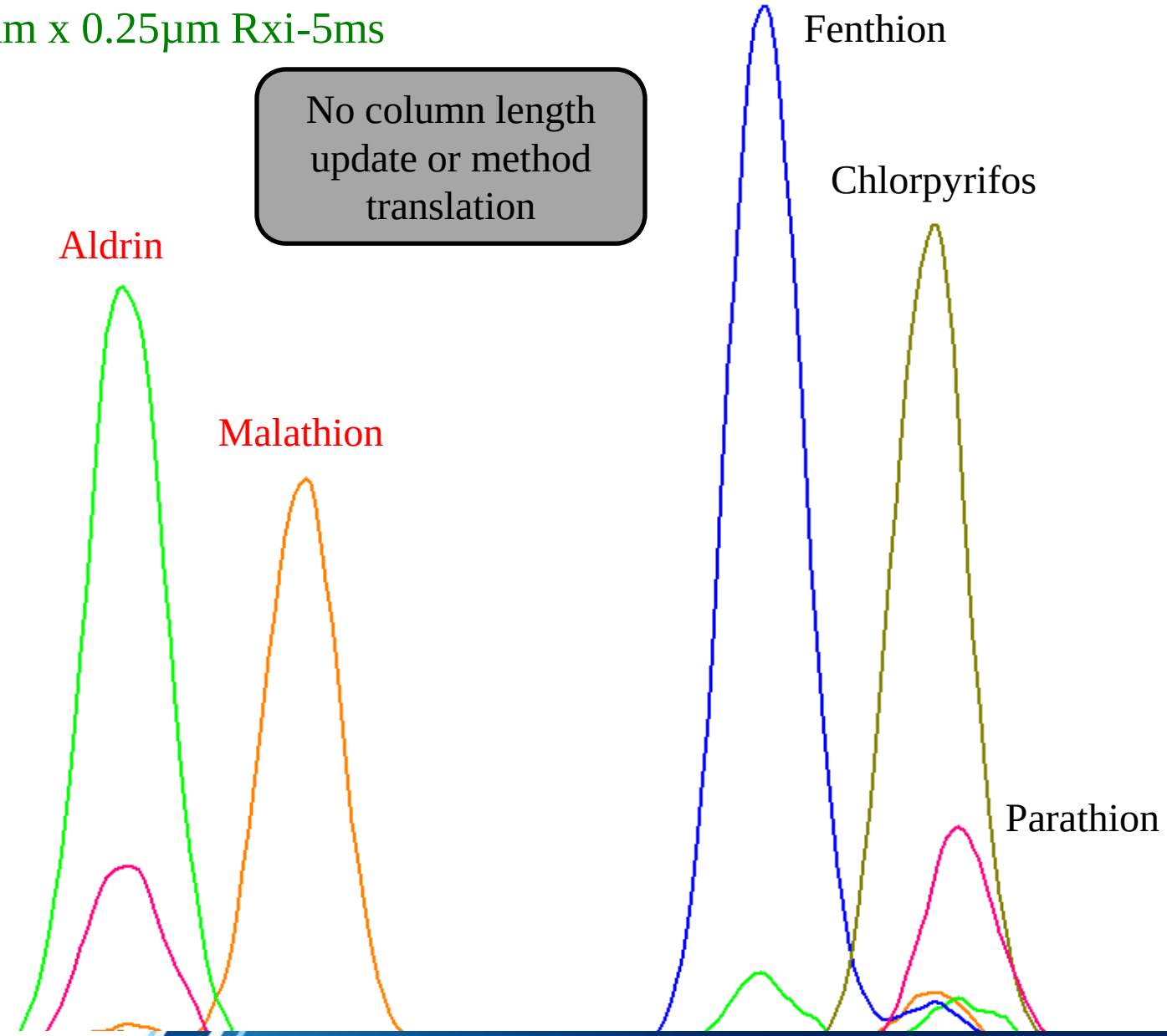
27.6m x 0.25mm x 0.25µm Rxi-5ms

No column length update or method translation



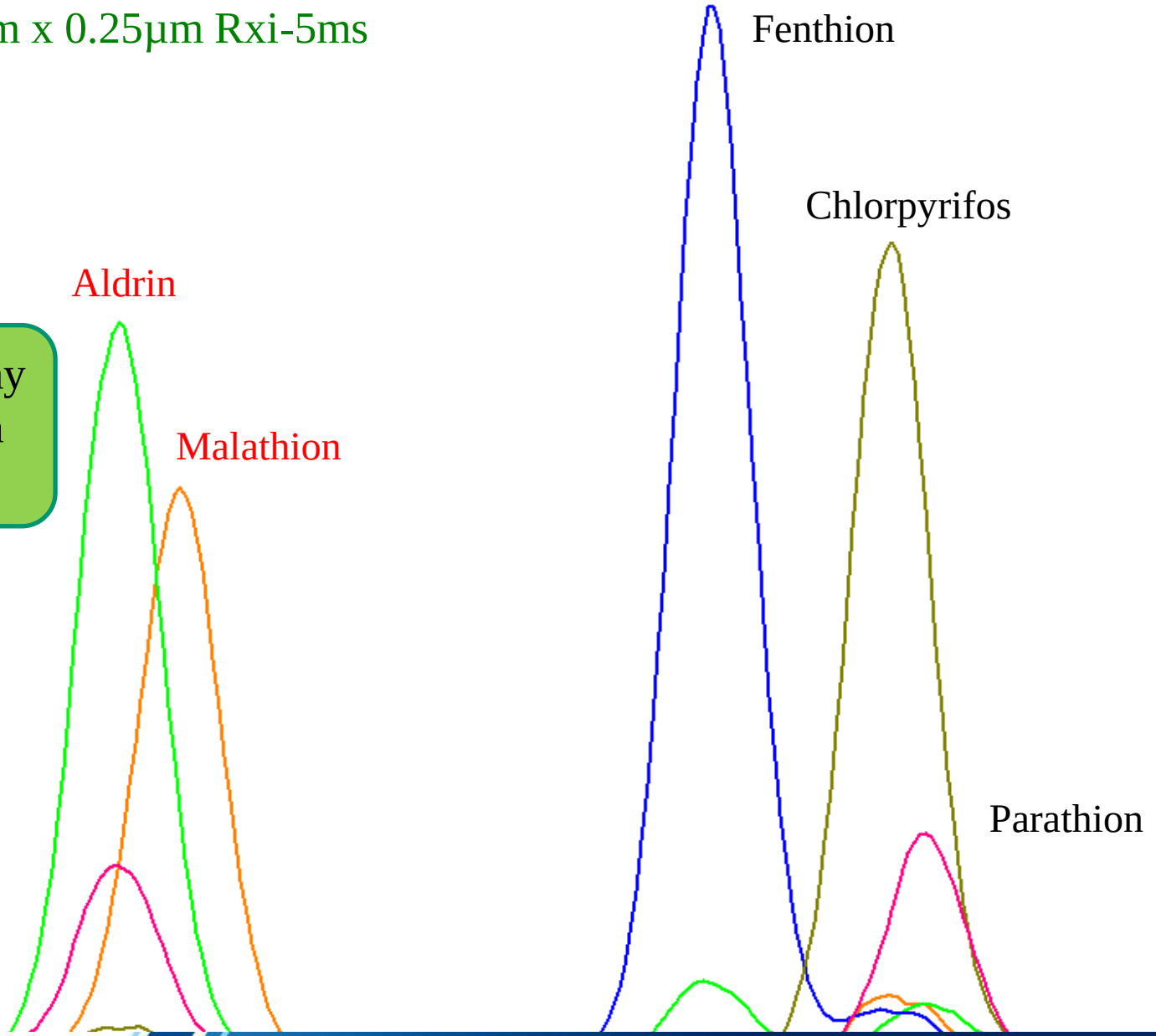
23.7m x 0.25mm x 0.25µm Rxi-5ms

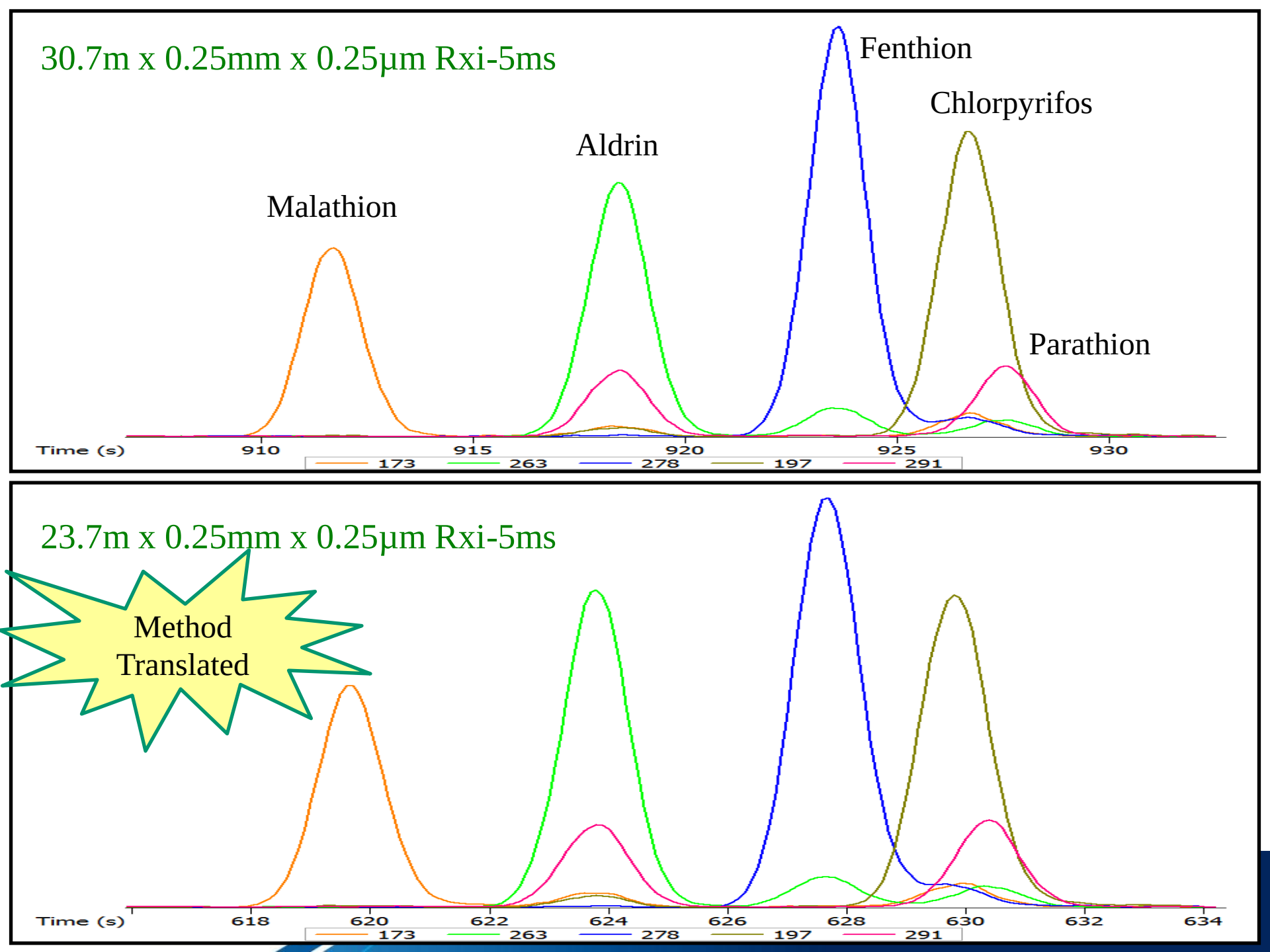
No column length update or method translation

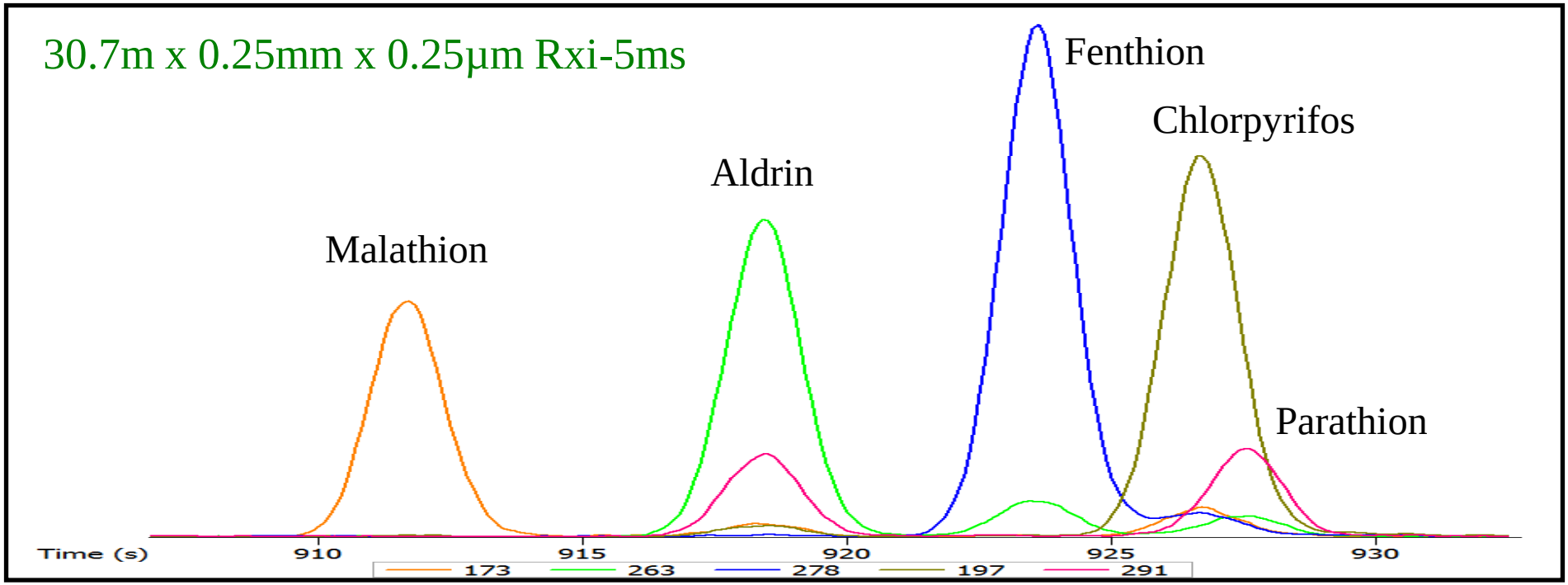


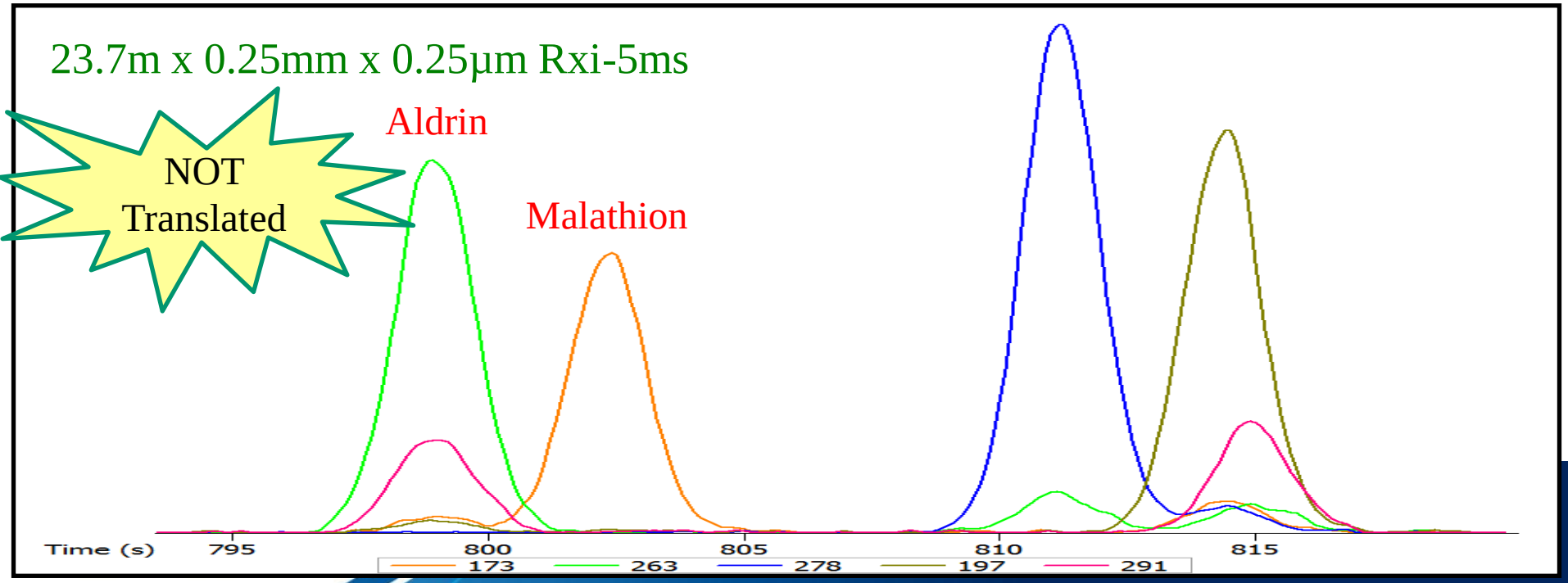
23.7m x 0.25mm x 0.25µm Rxi-5ms

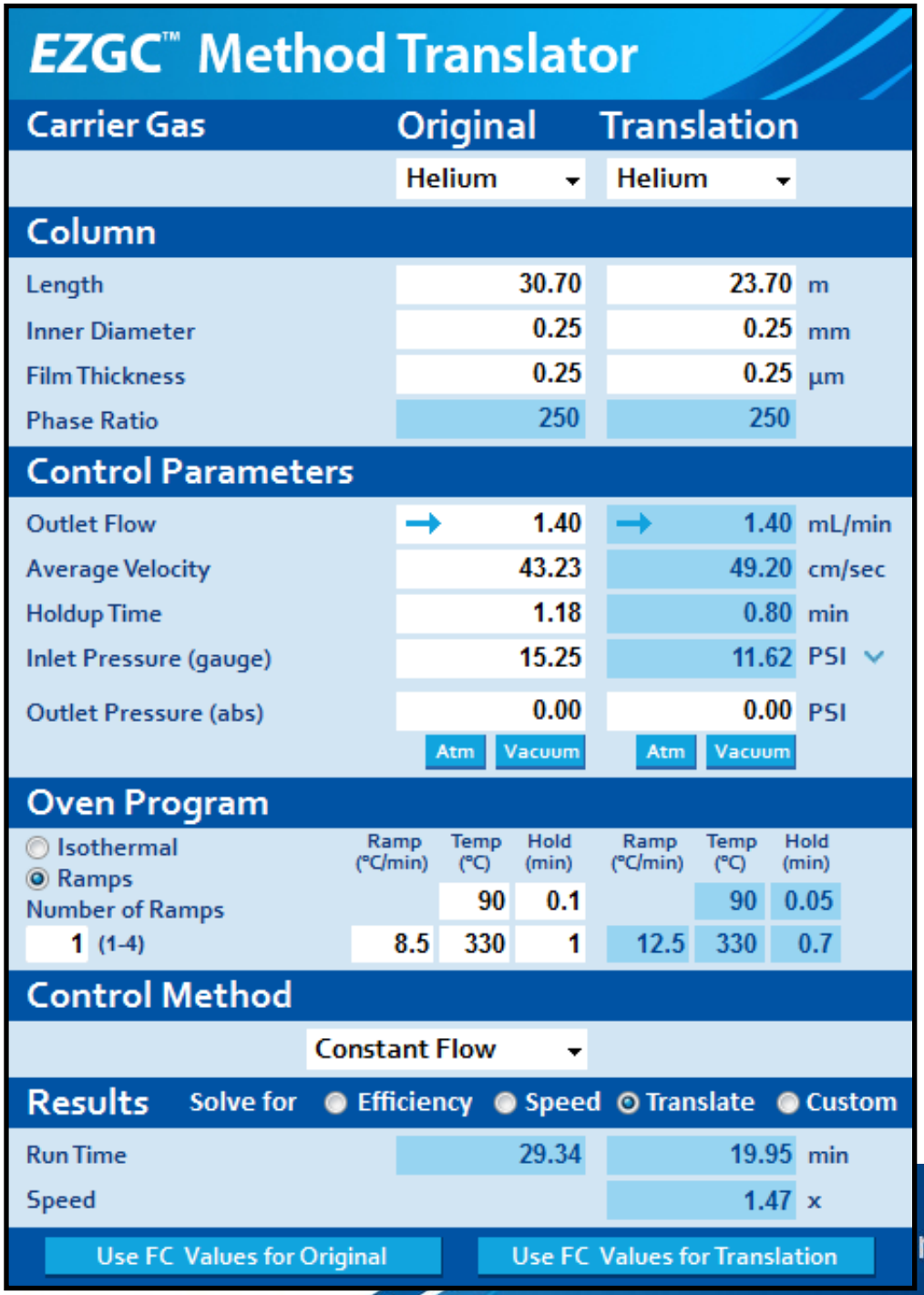
I will change my column length but that is IT!!



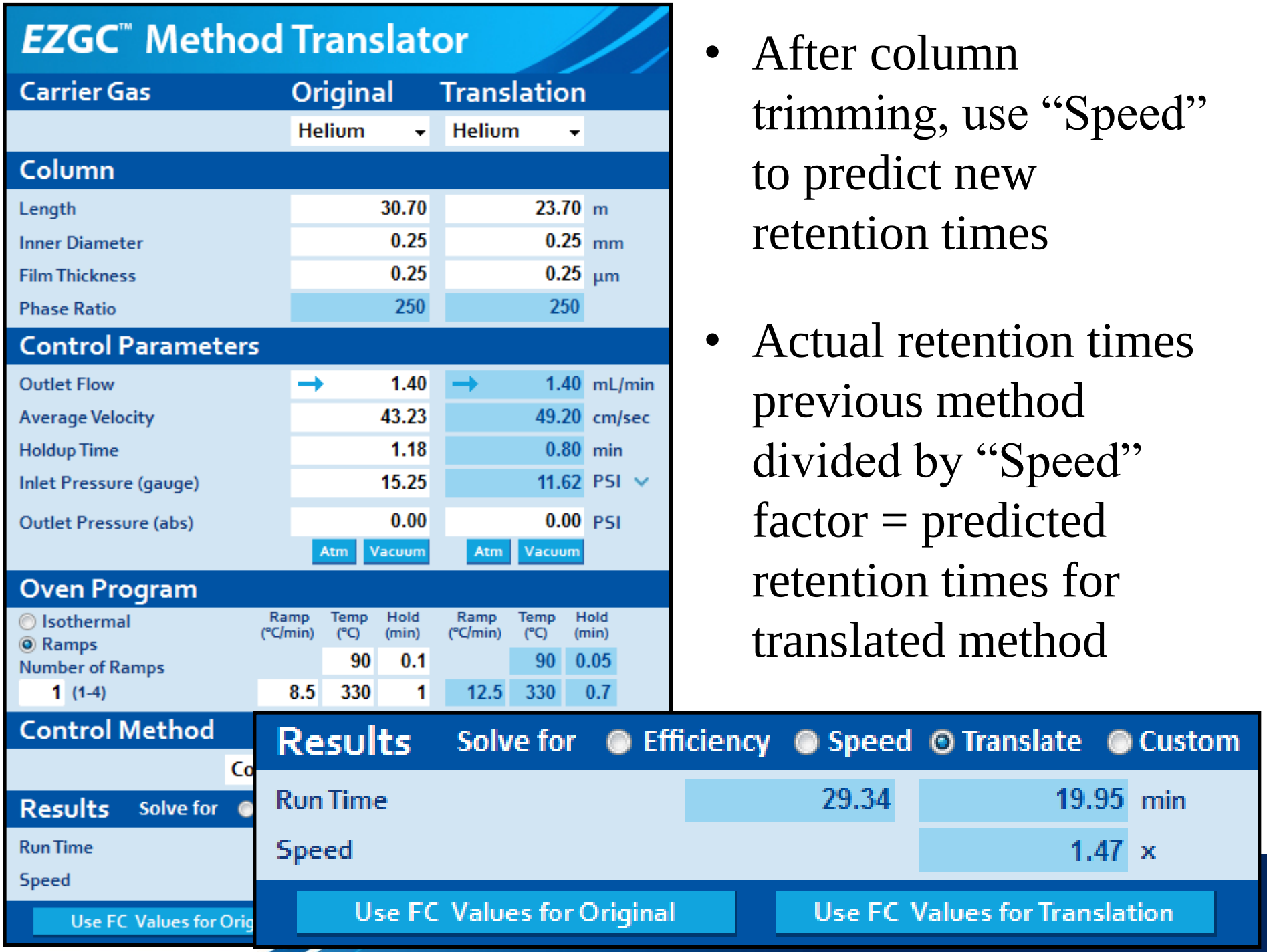

30.7m x 0.25mm x 0.25µm Rxi-5ms
Malathion
Aldrin
Fenthion
Chlorpyrifos
Parathion
Time (s)
910
915
920
925
930
173
263
278
197
291
23.7m x 0.25mm x 0.25µm Rxi-5ms
Method Translated
Time (s)
618
620
622
624
626
628
630
632
634
173
263
278
197
291


30.7m x 0.25mm x 0.25µm Rxi-5ms
Malathion
Aldrin
Fenthion
Chlorpyrifos
Parathion
Time (s)
910
915
920
925
930
173
263
278
197
291


23.7m x 0.25mm x 0.25µm Rxi-5ms
NOT Translated
Aldrin
Malathion
Time (s)
795
800
805
810
815
173
263
278
197
291




- After column trimming, use “Speed” to predict new retention times
- Actual retention times previous method divided by “Speed” factor = predicted retention times for translated method

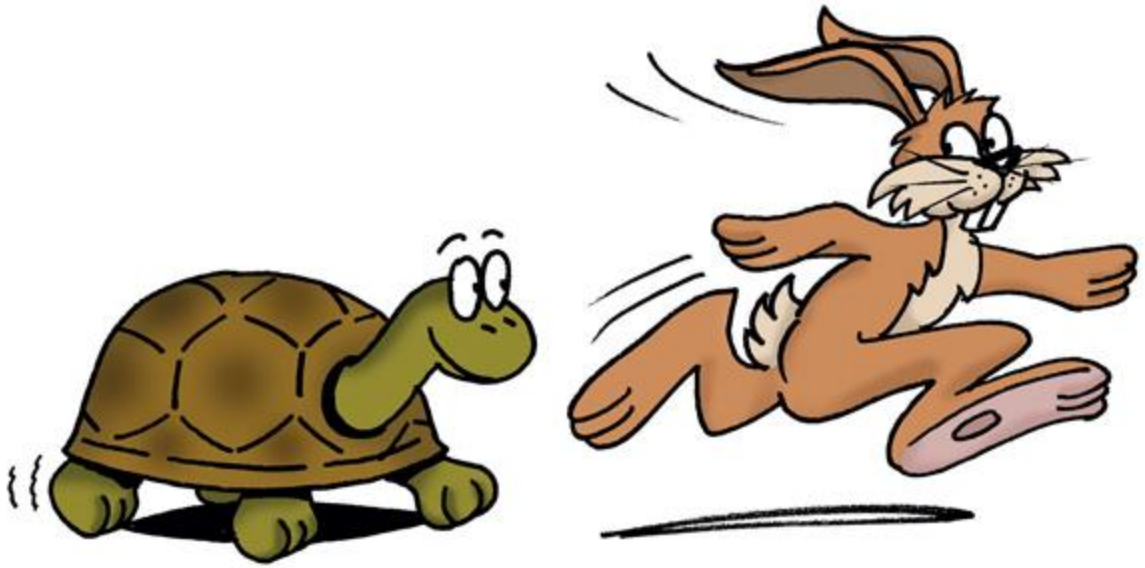



- After column trimming, use “Speed” to predict new retention times
- Actual retention times previous method divided by “Speed” factor = predicted retention times for translated method

# *EZ*GC™ Method Translator / Flow Calculator

Increasing speed of analysis

- Decreasing column L and/or ID
- Switching to a faster carrier gas (e.g., He to $H_2$)



# EZGC™ Method Translator

| Carrier Gas | Original | Translation | |
|---|---|---|---|
| | Helium | Helium | |
| **Column** | | | |
| Length | 30.70 | 20.10 | m |
| Inner Diameter | 0.25 | 0.18 | mm |
| Film Thickness | 0.25 | 0.18 | µm |
| Phase Ratio | 250 | 250 | |
| **Control Parameters** | | | |
| Outlet Flow | → 1.40 | → 1.01 | mL/min |
| Average Velocity | 43.23 | 45.33 | cm/sec |
| Holdup Time | 1.18 | 0.74 | min |
| Inlet Pressure (gauge) | 15.25 | 24.97 | psi |
| Outlet Pressure (abs) | 0.00 | 0.00 | psi |
| | Atm Vacuum | Atm Vacuum | |

**Oven Program**

Isothermal / Ramps — Number of Ramps: 1 (1-4)

| | Ramp (°C/min) | Temp (°C) | Hold (min) | Ramp (°C/min) | Temp (°C) | Hold (min) |
|---|---|---|---|---|---|---|
| | | 90 | 0.1 | | 90 | 0.05 |
| | 8.5 | 330 | 1 | 13.6 | 330 | 0.65 |

**Control Method**

Constant Flow

**Results** Solve for: Efficiency / Speed / Translate / Custom

| | | | |
|---|---|---|---|
| Run Time | 29.34 | 18.35 | min |
| Speed | | 1.60 | x |

Method Translator sets flow and oven rate for Translation column.

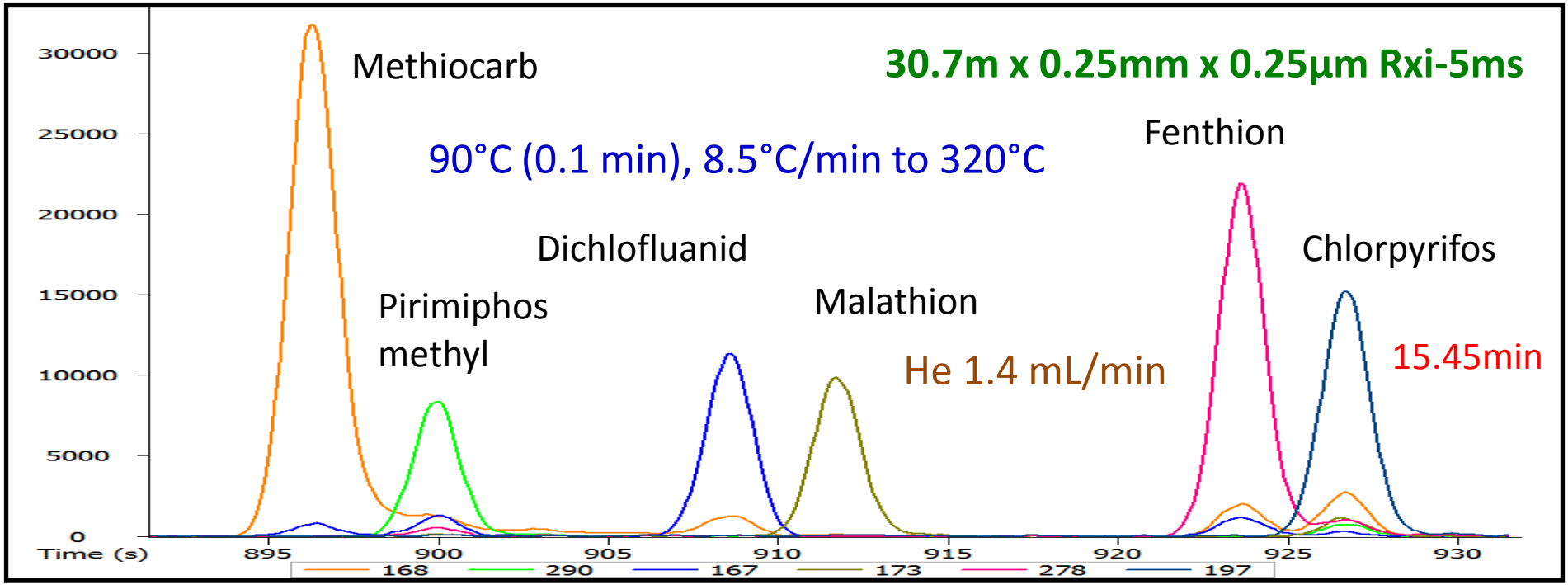
| | | | |
|---|---|---|---|
| | → 1.40 | → 1.01 | mL/min |
| | 43.23 | 45.33 | cm/sec |
| | 1.18 | 0.74 | min |
| | 15.25 | 24.97 | psi |
| | 0.00 | 0.00 | psi |
| | Atm Vacuum | Atm Vacuum | |

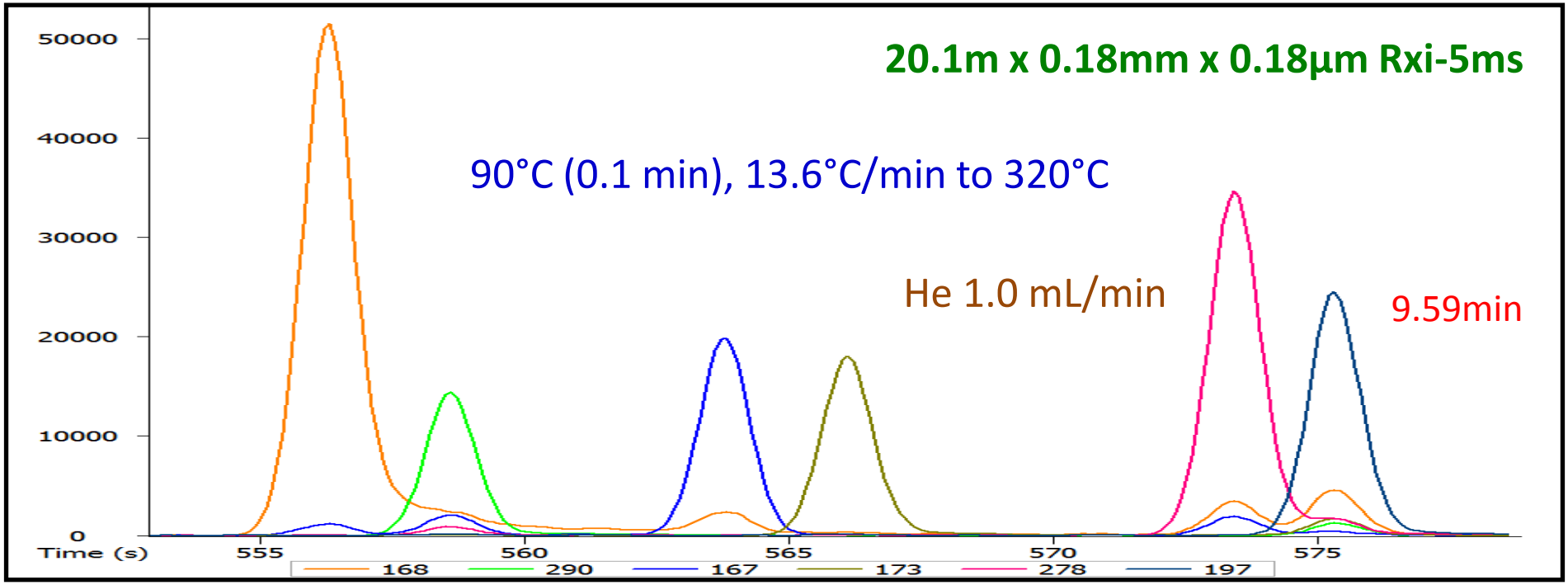
| Ramp (°C/min) | Temp (°C) | Hold (min) | Ramp (°C/min) | Temp (°C) | Hold (min) |
|---|---|---|---|---|---|
| | 90 | 0.1 | | 90 | 0.05 |
| 8.5 | 330 | 1 | 13.6 | 330 | 0.65 |

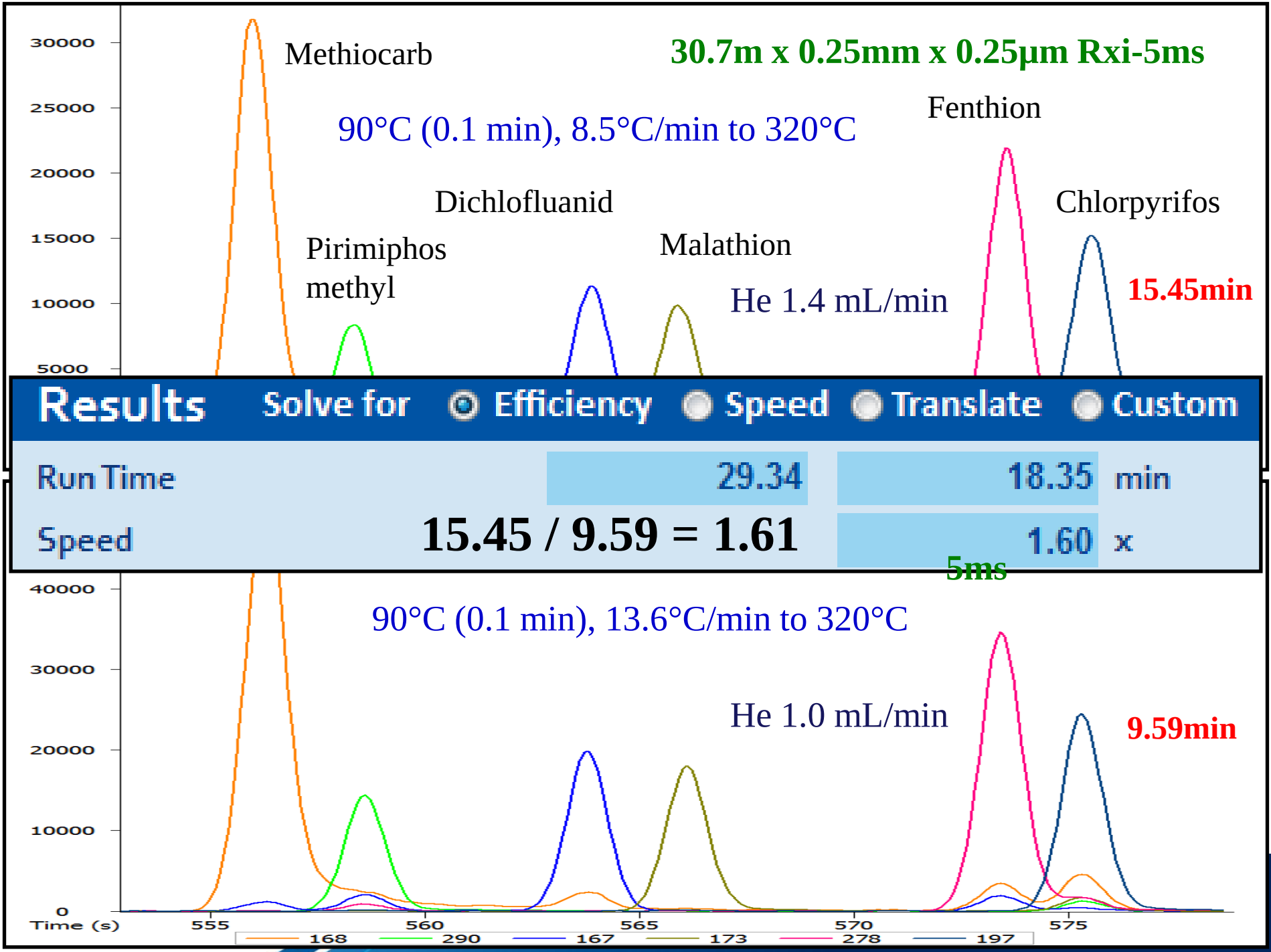
Constant Flow

Efficiency / Speed / Translate / Custom

| | | |
|---|---|---|
| 29.34 | 18.35 | min |
| | 1.60 | x |

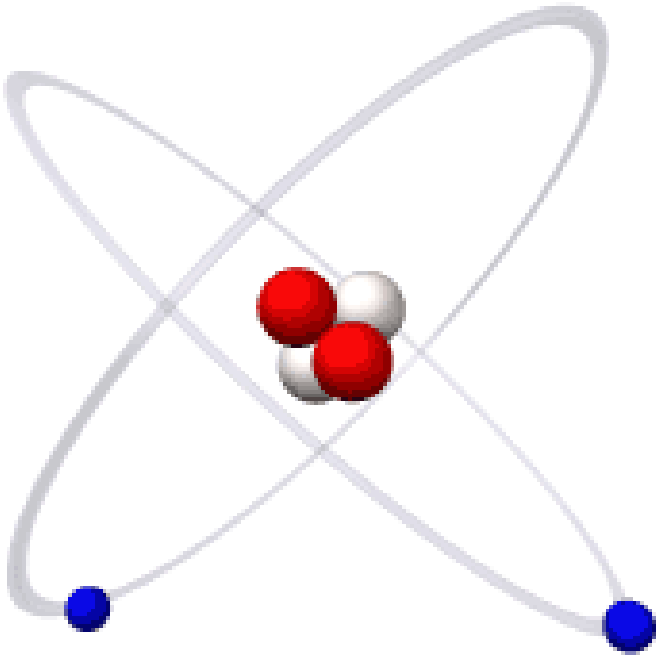

30000
25000
20000
15000
10000
5000
0
Time (s)
895
900
905
910
915
920
925
930
Methiocarb
30.7m x 0.25mm x 0.25µm Rxi-5ms
90°C (0.1 min), 8.5°C/min to 320°C
Fenthion
Dichlofluanid
Chlorpyrifos
Pirimiphos
methyl
Malathion
He 1.4 mL/min
15.45min
168
290
167
173
278
197

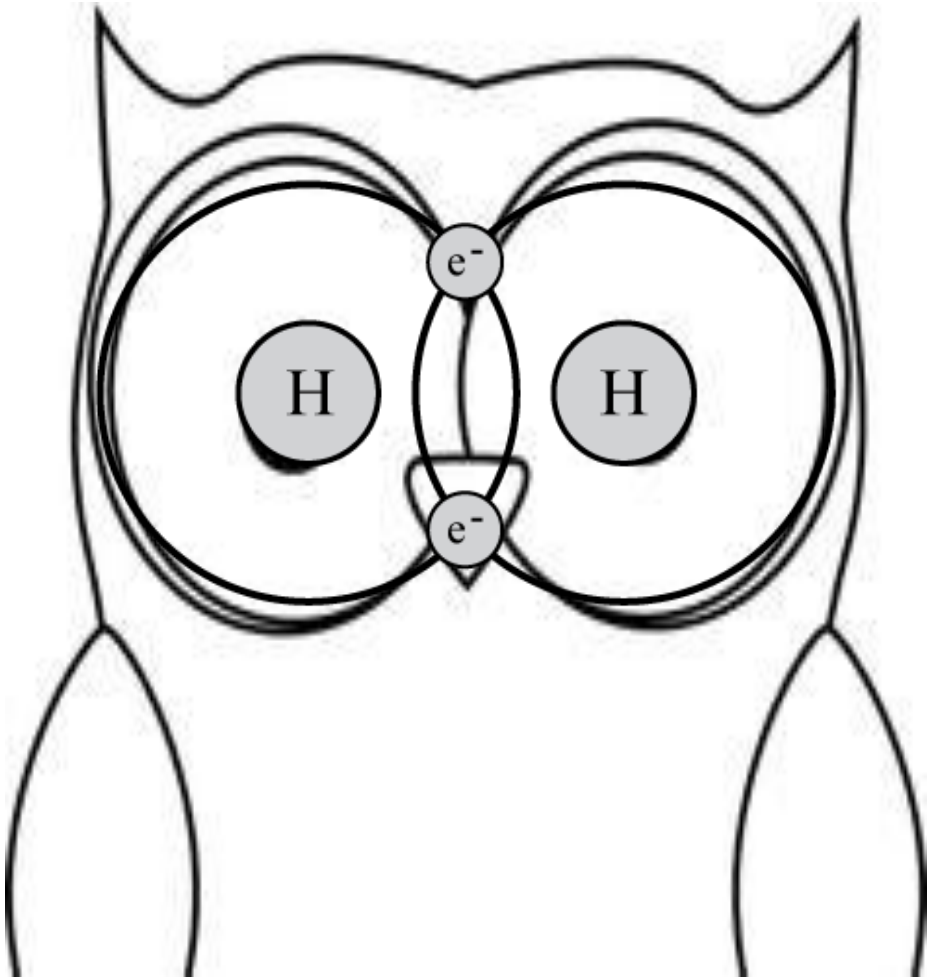

50000
40000
30000
20000
10000
0
Time (s)
555
560
565
570
575
20.1m x 0.18mm x 0.18µm Rxi-5ms
90°C (0.1 min), 13.6°C/min to 320°C
He 1.0 mL/min
9.59min
168
290
167
173
278
197

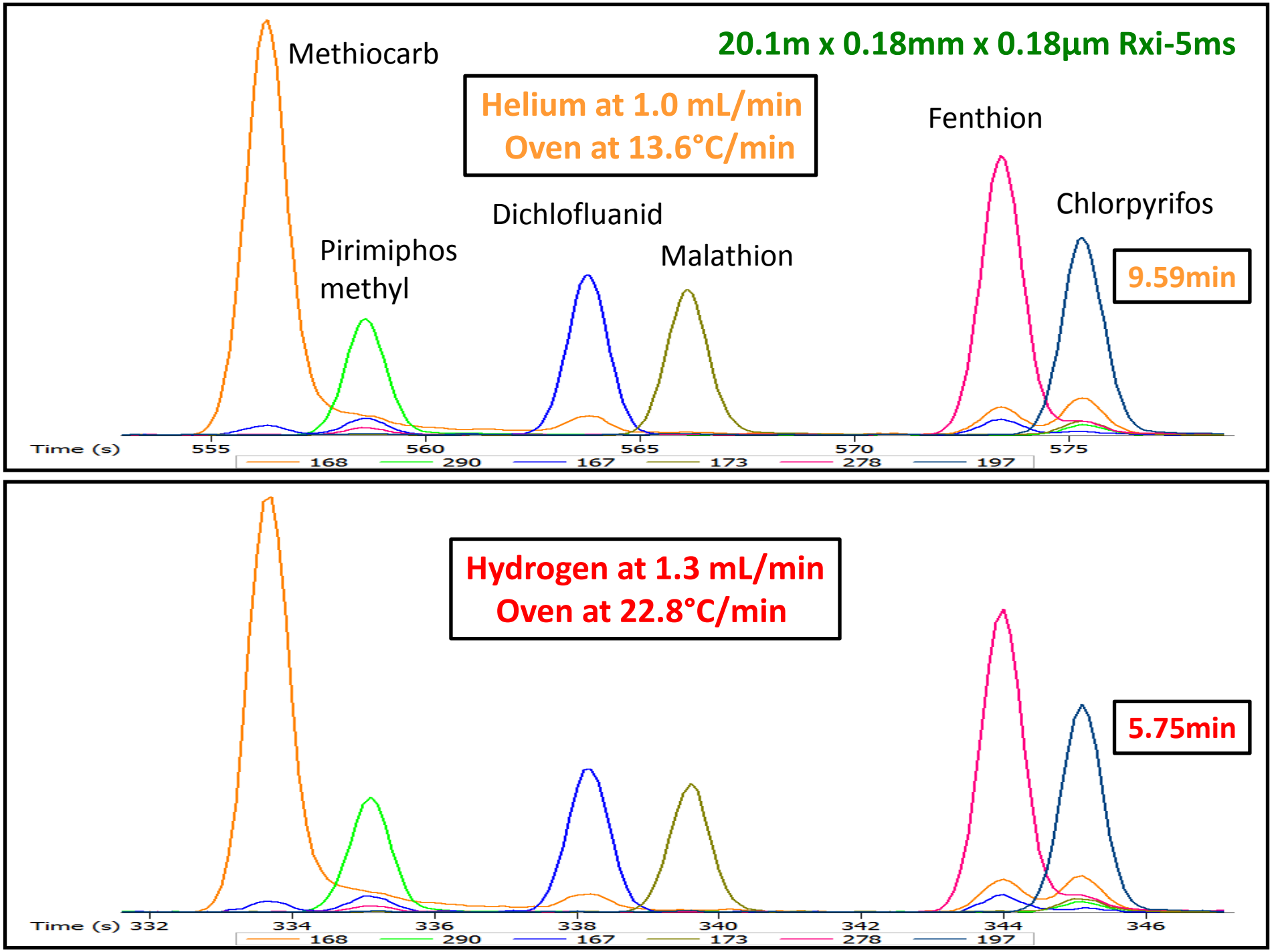

30000
25000
20000
15000
10000
5000
Methiocarb
30.7m x 0.25mm x 0.25µm Rxi-5ms
90°C (0.1 min), 8.5°C/min to 320°C
Fenthion
Dichlofluanid
Chlorpyrifos
Pirimiphos
methyl
Malathion
He 1.4 mL/min
15.45min
Results
Solve for
Efficiency
Speed
Translate
Custom
Run Time
29.34
18.35
min
Speed
15.45 / 9.59 = 1.61
1.60
x
5ms
40000
30000
20000
10000
0
90°C (0.1 min), 13.6°C/min to 320°C
He 1.0 mL/min
9.59min
Time (s)
555
560
565
570
575
168
290
167
173
278
197

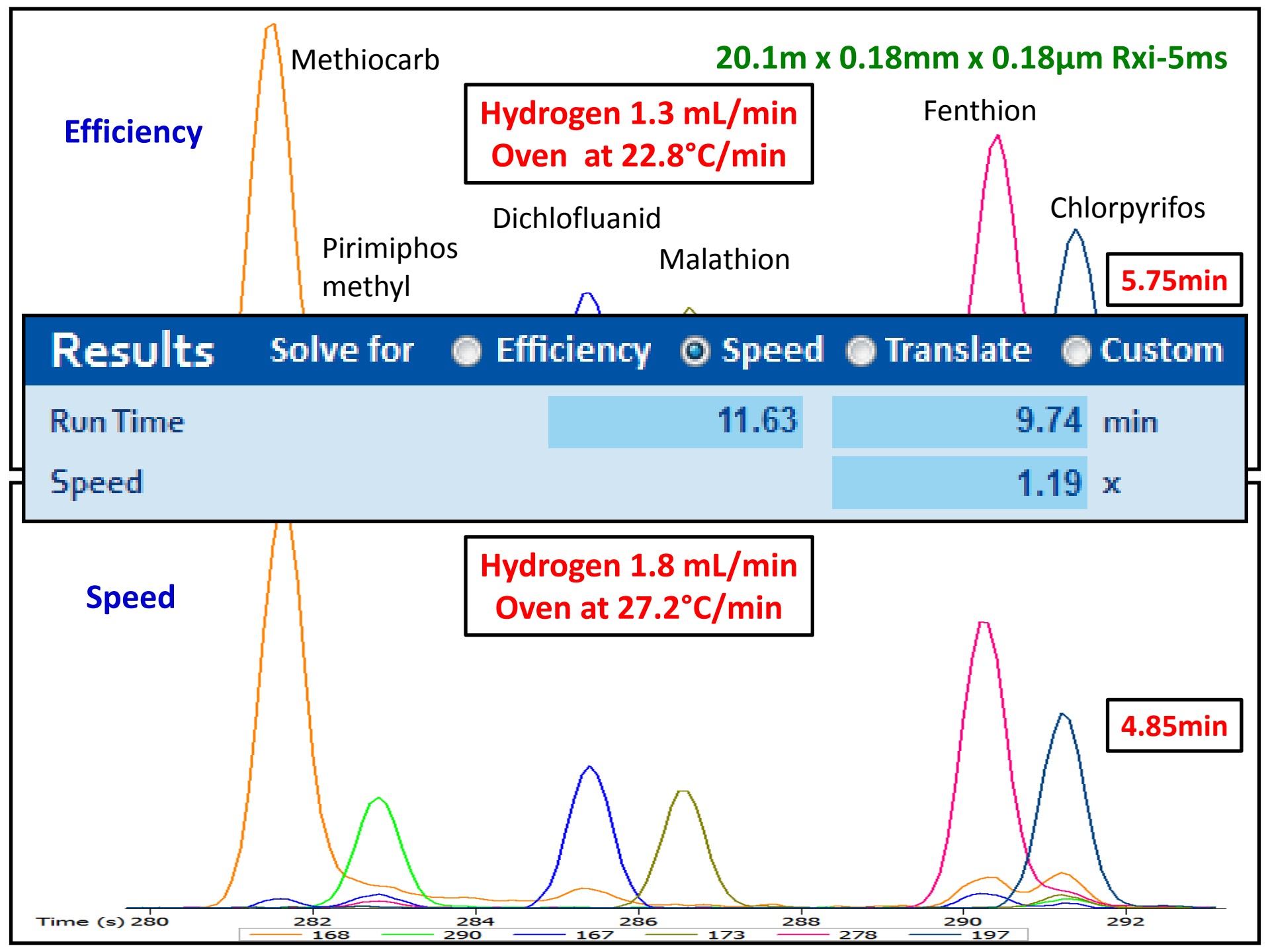
# Helium to Hydrogen Carrier Gas

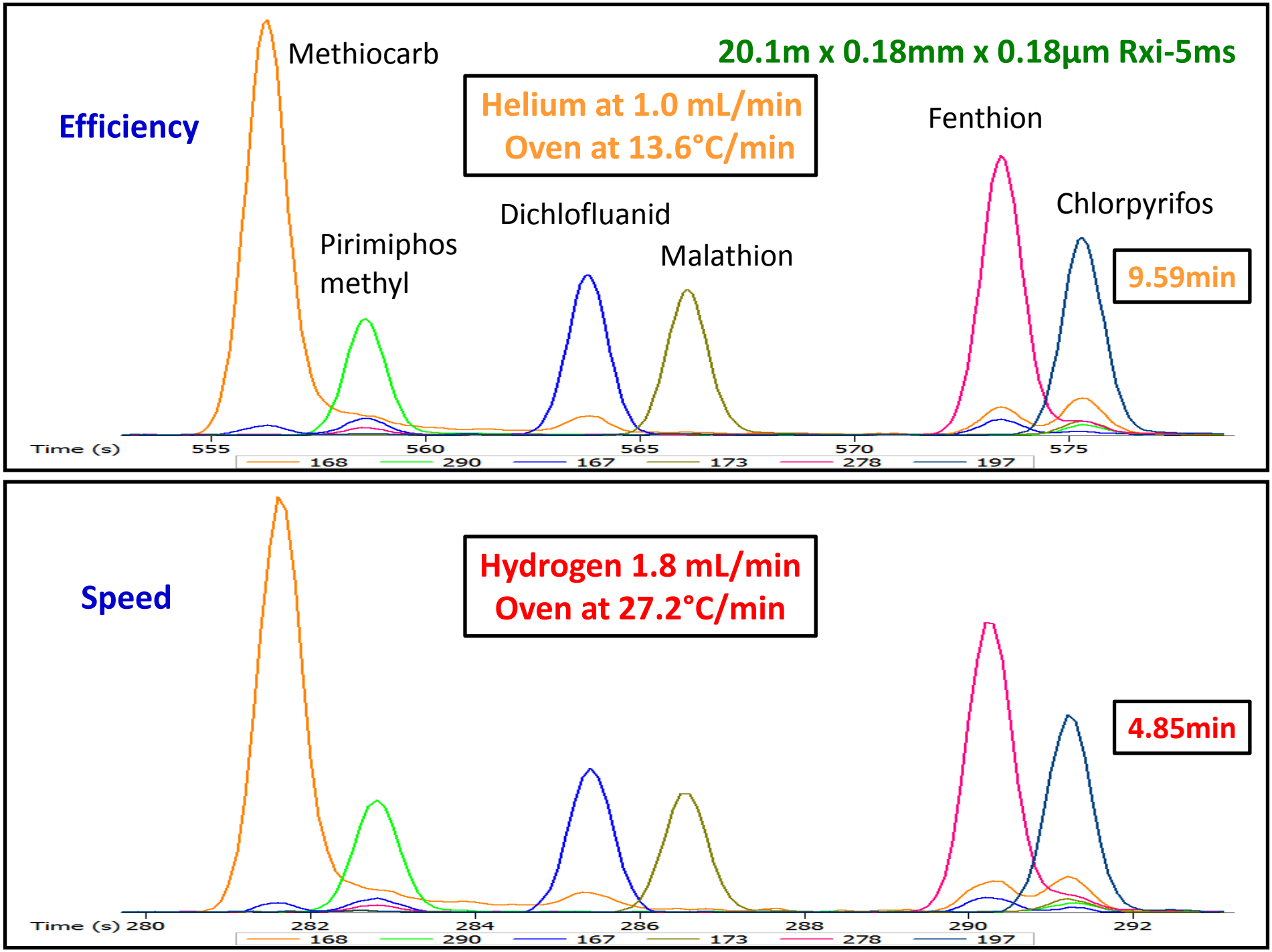
- 20m x 0.18mm x 0.18µm






20.1m x 0.18mm x 0.18µm Rxi-5ms
Methiocarb
Helium at 1.0 mL/min
Oven at 13.6°C/min
Fenthion
Dichlofluanid
Chlorpyrifos
Pirimiphos
methyl
Malathion
9.59min
Time (s)
555
560
565
570
575
168
290
167
173
278
197
Hydrogen at 1.3 mL/min
Oven at 22.8°C/min
5.75min
Time (s)
332
334
336
338
340
342
344
346
168
290
167
173
278
197


20.1m x 0.18mm x 0.18µm Rxi-5ms
Efficiency
Methiocarb
Hydrogen 1.3 mL/min
Oven at 22.8°C/min
Fenthion
Chlorpyrifos
Dichlofluanid
Pirimiphos
methyl
Malathion
5.75min
Results
Solve for
Efficiency
Speed
Translate
Custom
Run Time
11.63
9.74
min
Speed
1.19
x
Speed
Hydrogen 1.8 mL/min
Oven at 27.2°C/min
4.85min
Time (s) 280
282
284
286
288
290
292
168
290
167
173
278
197

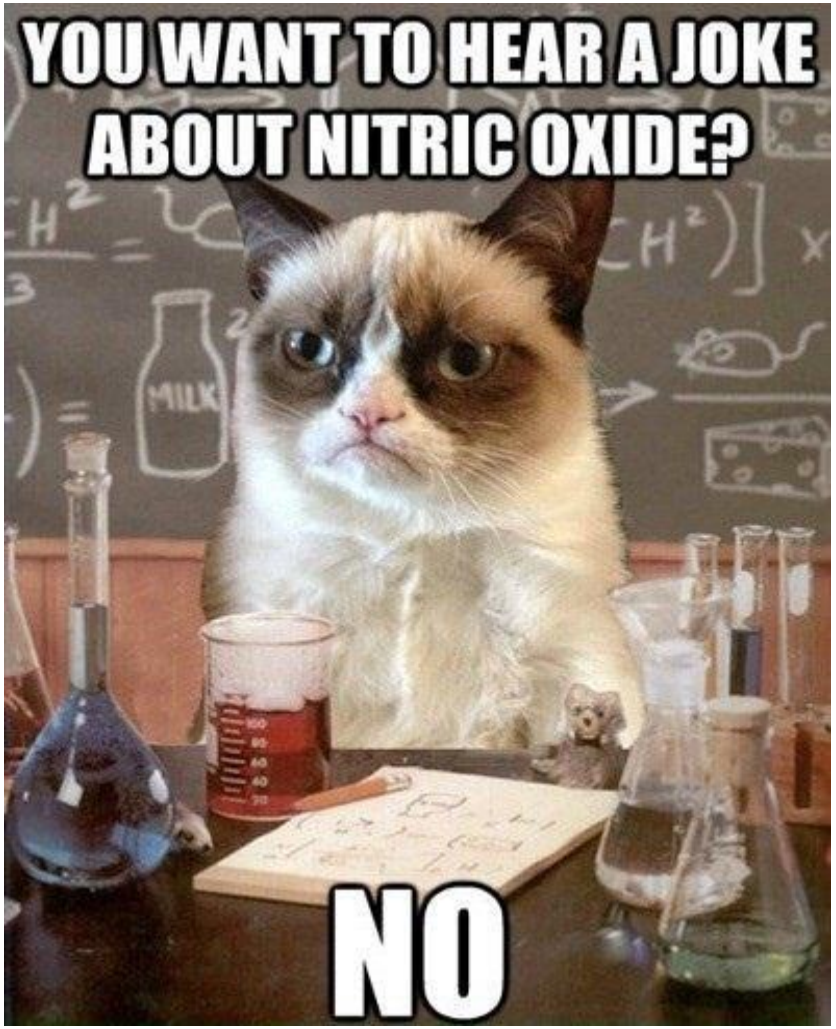

Efficiency
Methiocarb
20.1m x 0.18mm x 0.18µm Rxi-5ms
Helium at 1.0 mL/min
Oven at 13.6°C/min
Fenthion
Chlorpyrifos
Dichlofluanid
Pirimiphos methyl
Malathion
9.59min
Time (s)
555
560
565
570
575
168
290
167
173
278
197
Speed
Hydrogen 1.8 mL/min
Oven at 27.2°C/min
4.85min
Time (s)
280
282
284
286
288
290
292
168
290
167
173
278
197

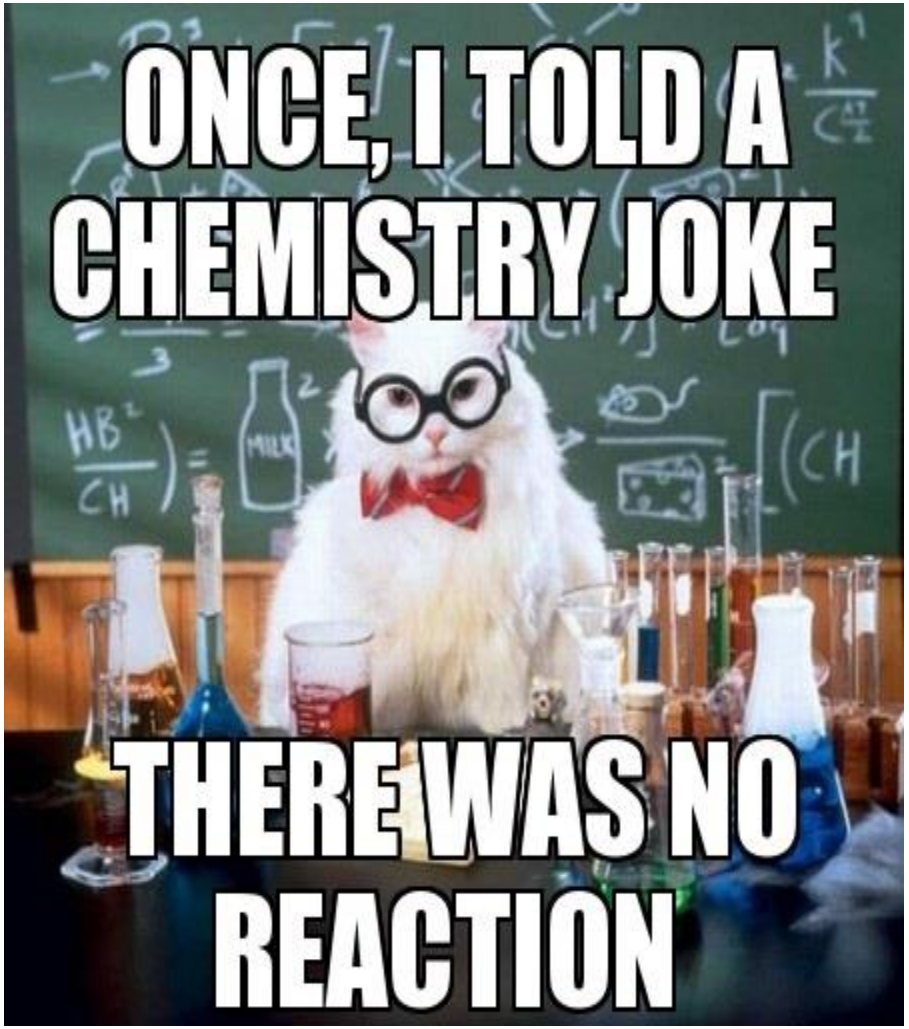
# Simplify Method Development

- ✓ SOF, EOF and OHR
- ✓ *EZ*GC Chromatogram Modeler
- ✓ *EZ*GC Flow Calculator
- ✓ *EZ*GC Method Translator

www.restek.com/Landing-Pages/EZGC-R-Method-Development-Tool-Suite

# THANK YOU!!

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