

## Flow rate calculation

$$F = Au_o = \frac{\pi d_c^2 \bar{u}}{4j}$$

$$u_o = \frac{\bar{u}}{j}$$

$$j = 1.5 \frac{\left(\frac{p_i}{p_o}\right)^2 - 1}{\left(\frac{p_i}{p_o}\right)^3 - 1}$$

- $d_c$  = column diameter
- $L$  = column length
- $p_i$  = inlet pressure
- $p_o$  = outlet pressure
- $U_o$  = outlet linear velocity

Example: on 30 m column, 100  $\mu\text{m}$  ID, an inlet gauge is set to 800 kPa, and outlet of column is assumed 101 kPa,  $t_M = 100\text{s}$  at  $100^\circ\text{C}$

Example: on 30 m column, 100  $\mu\text{m}$  ID, an inlet gauge is set to 800 kPa, and outlet of column is assumed 101 kPa,  $t_M = 100\text{ s}$ ,  $100^\circ\text{C}$

Then  $p_i = 901\text{ kPa}$  and  $p_o = 101\text{ kPa}$

$$j = 1.5 \frac{\left(\frac{p_i}{p_o}\right)^2 - 1}{\left(\frac{p_i}{p_o}\right)^3 - 1} = 1.5 \frac{\left(\frac{901}{101}\right)^2 - 1}{\left(\frac{901}{101}\right)^3 - 1} = 1.5 \frac{9^2 - 1}{9^3 - 1} = 1.5 \frac{80}{728} = 0.165$$

$$\bar{u} = \frac{L}{t_M} = \frac{3000}{100} = 30\text{ cm/s} \quad u_o = \frac{\bar{u}}{j} = \frac{30}{0.165} = 182\text{ cm/s} \quad \frac{p_o}{p_i} = \frac{u_i}{u_o}$$

$$F_c = Au_o = \frac{\pi d_c^2 \bar{u}}{4j} = \frac{3.14 \cdot 0.01^2 \cdot 30}{4 \cdot 0.165} = 0.014\text{ cm}^3/\text{s} = 0.86\text{ ml/min} \quad u_i = \frac{101}{901} 182 = 20.4\text{ cm/s}$$

$$F_a = \frac{T_c}{T_a} F_c = \frac{298}{373} 0.86 = 0.69\text{ ml/min}$$

$F_c$  outlet flow rate  
 $F_a$  actual flow rate (affected by temperature)  
 $F_{\text{incor}}$  + incorrect determination

$$F_{\text{incor}} = Au_o = \frac{\pi d_c^2 \bar{u}}{4} = \frac{3.14 \cdot 0.01^2 \cdot 30}{4} = 0.002\text{ cm}^3/\text{s} = 0.14\text{ ml/min}$$

# Injection Volume

- **Volume** Injected is Typically 0.1-3 $\mu$ L (liquid)
- **The injected volume is limited by the volume of solvent as a vapor phase.**

volume of vapor > then volume of injector results in backflash (system contamination)

*Solvent expansion volumes.*

Solvent	Density (g/mL)	MW	Expansion Volume in $\mu$ L at various column headpressures		
			5psig	10psig	15psig
Heptane	0.68	100	219	174	145
Hexane	0.66	86	245	196	163
Pentane	0.63	72	280	224	186
Toluene	0.87	92	303	242	201
Ethyl acetate	0.90	88	328	261	217
Chloroform	1.49	119	400	319	266
Methylene chloride	1.33	85	500	399	332
Methanol	0.79	32	792	629	525
H <sub>2</sub> O	1.00	18	1776	1418	1179

The expansion volumes were determined using a 1.0 $\mu$ L injection volume, a 250 $^{\circ}$  C injection port temperature, and a headpressure of 5, 10, or 15psig (common operating pressures for 30m columns having IDs of 0.53, 0.32, or 0.25mm, respectively). For 2 $\mu$ L injections, double the expansion volumes.

# Vapor volume

**Number of moles in injected volume**

$$n = \frac{m}{MW} = \frac{dV}{MW}$$

M = mass, MW = molecular weight, d = density

hexane

**Volume of the vapor**

$$V = \frac{nRT}{p} = \frac{n \cdot 8.31 \cdot T}{p_i + 101325}$$

$$n = \frac{0.66 \text{ g / mL} \cdot 10^{-3} \text{ mL}}{86 \text{ g / mol}} = 8.75 \cdot 10^{-6} \text{ mol}$$

1 psi = 6894 Pa

$$V = \frac{8.75 \cdot 10^{-6} \cdot 8.31 \cdot (273 + 250)}{5 \cdot 6894 + 101325} = 2.46 \cdot 10^{-7} \text{ m}^3 = 0.246 \text{ mL}$$

## How about acetonitrile

5 psii

d= 0.8 g/mL; MW =41

$$n = \frac{0.8 \text{ g / mL} \cdot 10^{-3} \text{ mL}}{41 \text{ g / mol}} = 1.95 \cdot 10^{-5} \text{ mol}$$

200°C

$$V = \frac{1.95 \cdot 10^{-5} \cdot 8.31 \cdot (200 + 250)}{5 \cdot 6894 + 101325} = 0.565 \text{ mL}$$

250°C

$$V = \frac{1.95 \cdot 10^{-5} \cdot 8.31 \cdot (250 + 250)}{5 \cdot 6894 + 101325} = 0.625 \text{ mL}$$

300°C

$$V = \frac{1.95 \cdot 10^{-5} \cdot 8.31 \cdot (300 + 250)}{5 \cdot 6894 + 101325} = 0.685 \text{ mL}$$

4 mm id, liner, L= 7 cm  $V = \pi r^2 L = 3.14 \cdot (0.2)^2 \cdot 7 \sim 0.9 \text{ mL}$

<http://www.chem.agilent.com/cag/main.html#flowcalc205>

The screenshot shows the 'Solvent Vapor Volume Calculator' window. At the top, it displays 'Approximate vapor volume(ul): 792 ul' and '80 %'. Below this is a progress bar. The main interface is divided into several sections:

- Injection Volume (ul):** A slider and input field set to 1.0.
- Inlet Temp (C):** A slider and input field set to 250.
- Inlet Pressure:** A slider and input field set to 5.
- Pressure Units:** Radio buttons for KPa, psi (selected), and bar.
- Solvent Properties:** A dropdown menu set to 'Methanol'. Below it, 'Boiling Pt (C): 64.7', 'Denisty (g/cm3): 0.791', and 'Mol Wt. (amu): 32' are listed. A 'Solvents' button with a flask icon is also present.
- Injection Liner:** A dropdown menu set to '19251-60540 strai' and 'Volume (ul): 990'.
- Capacity limits (%):** Two input fields set to 75 and 100.

Buttons for 'Print', 'Help', and 'OK' are located at the bottom left.