# Flow rate calculation

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

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

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

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

Example: on 30 m column, 100 µm ID, an inlet gauge is set to 800 kPa, and outlet of column is assumed 101 kPa, $t_M$ =100s at 100°C

## Example: on 30 m column, 100 µm ID, an inlet gauge is set to 800 kPa, and outlet of column is assumed 101 kPa, $t_M$ = 100 s, 100 °C

Then $p_i$=901 kPa and $p_o$=101 kPa

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

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

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

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

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

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

# Injection Volume

- **Volume** Injected is Typically 0.1-3µL (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 µL 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 |
| $H_2O$ | 1.00 | 18 | 1776 | 1418 | 1179 |

The expansion volumes were determined using a 1.0µL injection volume, a 250° 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 2µL 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

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

**Volume of the vapor**

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

1 psi = 6894 Pa

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

# How about acetonitrile

5 psii

d= 0.8 g/mL; MW =41

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

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

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

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

**4 mm id, liner, L= 7 cm V = $\pi r^2 L$ = 3.14.(0.2)².7~0.9mL**

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