Summary of equations (Bottcher)

System:

A ternary system composed of ammonia (1), oxygen (2) and nitrogen (3) is used by Bottcher (2009) in an axi-symmetric geometry.

1. Continuity equation or molar flux balance equation:

$$\nabla.\left(-D_{ij}\nabla C_i + C_i V\right) = 0 \tag{1}$$

Where, C_i is the concentration in kg/m^3.

Note: the continuity equation given in the article is $\nabla.(\rho V) = 0$. However, COMSOL did not exhibit convergence.

When expanded equation (1) takes the following form for component 1,

$$(D_{12} + D_{13})(\frac{\partial^2 C_1}{\partial x^2} + \frac{\partial^2 C_1}{\partial y^2}) = C_1\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + u\left(\frac{\partial C_1}{\partial x}\right) + v\left(\frac{\partial C_1}{\partial y}\right) \tag{2}$$

Here, u and v are the x and y components of the velocity vector.

Similar equations can be derived for components 2 and 3.

2. Stefan-Maxwell equations:

$$u.\nabla \mathrm{w_i} = -\frac{1}{\rho}\nabla.\left(\frac{\rho M_i}{{M_{av}}^2}\sum_{j=1,j\neq i}^{N} M_j D_{ij}\nabla x_j\right) \tag{3}$$

Here, $\mathrm{w_i}$ denotes the weight/mass fraction of component i, which is related to mole fraction in the following manner:

$$x_i = w_i\frac{M_{av}}{M_i} \tag{4}$$

On substituting (3) in (4) and expanding, we get, for component 1, we have

$$\rho\left(\frac{M_1}{M_{av}}\right)\left(u\frac{\partial x_1}{\partial x} + v\frac{\partial x_1}{\partial y}\right) = \nabla.(\rho\left(\frac{M_1}{M_{av}^2}\right)(M_2 D_{12}\nabla \mathrm{x_2} + M_3 D_{13}\nabla \mathrm{x_3})\,) \tag{5}$$

Equation (5) is separated into x and y components.

The system density is given by:

$$\rho = \left(1 - \sum_{i=1}^{N-1} w_i\right)\rho_N + \sum_{i=1}^{N-1} w_i\,\rho_i \tag{6}$$

This equation is again changed in terms of the mole fractions as follows:

$$\rho = \frac{1}{M_{av}}\left(\rho_1 M_1 x_1 + \rho_2 M_2 x_2 + \rho_3 M_3 x_3\right) \tag{7}$$

According to Bottcher (2009), the diffusivities used in equation (5) are not the binary diffusivities. The dependence of diffusivity on weight fractions is presented in the article. For the sake of convenience in modeling, this dependence was exhibited in terms of mole fractions. For instance,

$$D_{12} = d_{12}\left(1 + \frac{x_3\left(\frac{M_3\,d_{13}}{M_2} - d_{12}\right)}{x_1 d_{23} + x_2 d_{13} + x_3 d_{12}}\right) \tag{8}$$

And so on for other diffusivities.

The average molecular weight is represented using the following equation:

$$M_{av} = M_1 x_1 + M_2 x_2 + M_3 x_3 \tag{9}$$

3. Navier-Stokes equations:

The general form defined in the article is:

$$u.\nabla u = -\frac{1}{\rho}\,\nabla P + \frac{\eta}{\rho}\,\nabla.(\nabla u) + \frac{1}{3}\frac{\eta}{\rho}\,\nabla(\nabla.u) \tag{10}$$

This form is split into its x and y co-ordinates according to the convention used by Bird et.al. (2002).

x-component of momentum:

$$\rho(u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}) = -(\nabla P)_x + \frac{4}{3}(\eta)\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right) + \eta\left(\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial y}\right)\right) \tag{11}$$

y-component of momentum:

$$\rho(u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}) = -(\nabla P)_y + \frac{4}{3}(\eta)\frac{\partial}{\partial y}\left(\frac{\partial v}{\partial y}\right) + \eta\left(\frac{\partial}{\partial x}\left(\frac{\partial v}{\partial x}\right)\right) \quad (12)$$

The average viscosity η is assumed to be constant by the author. I have used the following approximation in COMSOL.

$$\eta = \frac{1}{3}(\eta_1 + \eta_2 + \eta_3) \quad (13)$$

Assumptions:

While solving equation (5) in COMSOL, following assumptions are made:

1. The system density,ρ, average molecular weight, M_{av} and the diffusivities D_{ij} are independent of the x and y positions. However, they depend on the mole fractions as per equations (7), (8) and (9).

3. The total pressure gradient is assumed to be zero, in both x and y directions. It can be justified based on the ideal gas law in the following way:

$$\nabla P = \nabla(CRT) = RT\nabla(C)$$

Since the total concentration is constant, gradient of concentration can be taken as zero in both the directions

The input radial velocity is given by the following equation:

$$v_0(r) = \frac{V_0}{2\pi F(R_{min,}R_{max})}(r - R_{min})(R_{max} - r) \quad (14)$$

In the above equation, V_0 is the input gas flow rate in Standard Cubic Centimeter minutes (SCCM) and R_{min} and R_{max} are the annular radii.

The function $F(R_{min,}R_{max})$ is given in the following manner:

$$F(R_{min,}R_{max}) = \frac{R_{min}^4 - R_{max}^4}{4} + \frac{R_{max}^3 - R_{min}^3}{3}(R_{min} + R_{max}) + \frac{R_{min}^2 - R_{max}^2}{2}(R_{min}R_{max}) \quad (15)$$

Parameters:

Parameter	Value
T	298 K
P	101325 Pa
$d_{12} = d_{13} = d_{23}$	0.1×10^{-4} m^2/s
R_{min}	7 cm
R_{max}	8 cm
V_0	280 sccm (standard cubic centimeters per minute)
$(\eta_1 = \eta_2 = \eta_3)$	1×10^{-5} Pa.s
$F(R_{min}, R_{max})$	1.25

Using the parameters, the input radial velocity expression can be further simplified:

$$v_0(r) = 59.41(r - 0.07)(0.08 - r) \tag{16}$$

Reference:

Bird, R., Stewert, W., Lightfoot, E., 2002. Transport Phenomena. John Wiley, New York.