In [19]:

```
from sympy import *
import matplotlib.pyplot as plt
init_printing()
```

Wmax

- for maximum plume length y = 0
- erf(x) is in scipy.special have to import from there
- erf(x) is also a part of sympy function.
- erf$(-x)$ = -erf(x): It is an odd function

We begin with eq (9) of the WRR paper, which is

$$C(x,y,z) = \frac{2}{\pi}(\gamma C_D^\circ + C_A^\circ)\left[\text{erf}\left(\frac{y+W}{\sqrt{4\alpha_{Th}x}}\right) - \text{erf}\left(\frac{y-W}{\sqrt{4\alpha_{Th}x}}\right)\right] \cdot \sum_{n=1}^{\infty}\frac{1}{(2n-1)}\exp\left(-\alpha_{Tv}\,x\,(\pi/2M)^2\right)\sin\left((2n-1)\frac{\pi z}{2M}\right) - C_A^\circ - C^* = 0 \tag{1}$$

Let $A = (\gamma C_D^\circ + C_A^\circ)$, $n = 1$ and $z = M$ (invariant), eq 1 then becomes

$$C(x,y,M) = \frac{2}{\pi}A\left[\text{erf}\left(\frac{y+W}{\sqrt{4\alpha_{Th}x}}\right) - \text{erf}\left(\frac{y-W}{\sqrt{4\alpha_{Th}x}}\right)\right] \cdot \exp\left(-\alpha_{Tv}\,x\,(\pi/2M)^2\right)\sin\left(\frac{\pi}{2}\right) - C_A^\circ - C^* = 0 \tag{2}$$

$\sin(\pi/2) = 1$, so eq 2 becomes

$$C(x,y,M) = \frac{2}{\pi}A\left[\text{erf}\left(\frac{y+W}{\sqrt{4\alpha_{Th}x}}\right) - \text{erf}\left(\frac{y-W}{\sqrt{4\alpha_{Th}x}}\right)\right] \cdot \exp\left(-\alpha_{Tv}\,x\,(\pi/2M)^2\right) - C_A^\circ - C^* = 0 \tag{3}$$

Let $B = \frac{\pi^2}{4M^2}\alpha_{Tv}$ and let $D = (C_A^\circ + C^*)$ then eq 3 becomes

$$C(x,y,M) = \frac{2}{\pi}A\left[\text{erf}\left(\frac{y+W}{\sqrt{4\alpha_{Th}x}}\right) - \text{erf}\left(\frac{y-W}{\sqrt{4\alpha_{Th}x}}\right)\right] \cdot \exp(-Bx) - D = 0 \tag{4}$$

Eq. (4) can be rewritten as:

$$\frac{2}{\pi}A\left[\text{erf}\left(\frac{y+W}{\sqrt{4\alpha_{Th}x}}\right) - \text{erf}\left(\frac{y-W}{\sqrt{4\alpha_{Th}x}}\right)\right] \cdot \exp(-Bx) = D \tag{5}$$

In [28]:

```
x,y,M, W, ath,A, B, C, D =symbols('x, y, M, W, ath, A, B, C, D')
```

In [32]:

```
eq4 = 2/pi*A*(erf((y+W)/sqrt(4*ath*x))-erf((y-W)/sqrt(4*ath*x)))*exp(-B*x)- D
```

The total derivative of left side of eq (4), with respect to x is

$$\frac{\partial C(x,y,M)}{\partial x}=\frac{\partial C(x)}{\partial x}\frac{dx}{dx}+\frac{\partial C(y)}{\partial y}\frac{dy}{dx}+\frac{\partial C(M)}{\partial M}\frac{dM}{dx} \tag{6}$$

in which M is invariant with respect to x, so $\frac{dM}{dx}=0$ and as a requirement for the maximum width, which is along y, $\frac{dy}{dx}=0$ has to be set. Thus, we have only $\frac{\partial C(x)}{\partial x}=0$, unsolved left in (5). Next, we obtain that

In [34]:

```
eq6 = diff(eq4, x) # dc/dx
```

$$-\frac{2AB\left(-\operatorname{erf}\left(\frac{-W+y}{2\sqrt{athx}}\right)+\operatorname{erf}\left(\frac{W+y}{2\sqrt{athx}}\right)\right)\exp(-Bx)}{\pi}+\frac{2A\left(\frac{\left(-\frac{W}{2}+\frac{y}{2}\right)\exp\left(-\frac{(-W+y)^2}{4athx}\right)}{\sqrt{\pi x}\sqrt{athx}}-\frac{\left(\frac{W}{2}+\frac{y}{2}\right)\exp\left(-\frac{(W+y)^2}{4athx}\right)}{\sqrt{\pi x}\sqrt{athx}}\right)\exp(-Bx)}{\pi}=0 \tag{7}$$

Using eq (5), eq (7) can be simplified to

$$-BD+\frac{2A}{\pi}\left(\frac{\left(-\frac{W}{2}+\frac{y}{2}\right)e^{-\frac{(-W+y)^2}{4athx}}}{\sqrt{\pi x}\sqrt{athx}}-\frac{\left(\frac{W}{2}+\frac{y}{2}\right)e^{-\frac{(W+y)^2}{4athx}}}{\sqrt{\pi x}\sqrt{athx}}\right)e^{-Bx}=0 \tag{8}$$

Eq. (4) and eq. (8) are two identical non-linear equations with two unknowns (x and y). Simultaneous solution of these two equations will provide the co-ordinate of the position of maximum width.

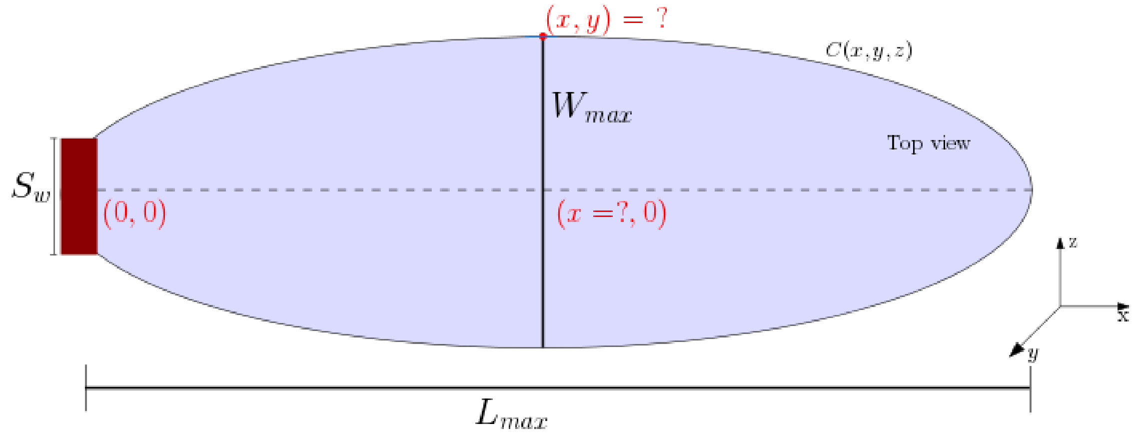
Solving strategy

Numerical methods has to be applied. Good initial value can be $x=L/2$ and $y=W$. These can be obtained from the 3D model. Numerical methods to check:

1. **Sympy** based Symbolic algorithms ***solve*** and ***nsolve*** algorithms (check flags, e.g. Force= True, manual = True etc). This can provide a direct solution.
2. **Scipy** algorithms ***fsolve***, ***root*** and non-linear solvers: ***Newton Krylov (JFNK)*** method, ***Broyden1*** method.

01 Tasks Update - W_{max} Solution

The problem Statement:



For the given *C (x,y,z) (3D model, Liedl et al. (2011):*

$$\mathbf{C}(\mathbf{x},\mathbf{y},\mathbf{z}) = \frac{2}{\pi}(\gamma C_D^\circ + C_A^\circ)\left[\mathrm{erf}\left(\frac{y+W}{\sqrt{4\alpha_{Th}x}}\right) - \mathrm{erf}\left(\frac{y-W}{\sqrt{4\alpha_{Th}x}}\right)\right]$$
$$\cdot \sum_{n=1}^{\infty} \frac{1}{(2n-1)} e^{\left(-\alpha_{Tv}\, x\, (\pi/2M)^2\right)} \sin\left((2n-1)\frac{\pi z}{2M}\right) - C_A^\circ - C^* = 0$$

What is the value of *(x,y)*?

01 Tasks Update - W_{max} Solution

***(x, y)* – two information are required, so the following two equations are obtained (based on Liedl et al., 2011) that may solve the problem:**

$$\frac{2}{\pi}A\left[\operatorname{erf}\left(\frac{y+W}{\sqrt{4\alpha_{Th}\,x}}\right)-\operatorname{erf}\left(\frac{y-W}{\sqrt{4\alpha_{Th}\,x}}\right)\right]\cdot e^{(-Bx)}-D=0$$ **Eq. 1**

$$-BD+\frac{2A}{\pi}\left(\frac{\left(-\frac{W}{2}+\frac{y}{2}\right)e^{-\frac{(-W+y)^2}{4ath\,x}}}{\sqrt{\pi}x\sqrt{ath\,x}}-\frac{\left(\frac{W}{2}+\frac{y}{2}\right)e^{-\frac{(W+y)^2}{4athx}}}{\sqrt{\pi}x\sqrt{ath\,x}}\right)e^{(-Bx)}=0$$ **Eq. 2**

With,

$$A=(\gamma C_D^\circ + C_A^\circ)$$

$$B=\frac{\pi^2}{4M^2}\alpha_{Tv}$$

$$D=(C_A^\circ + C^*)$$

Eq. (1) and Eq. (2) are a set of 2 non-linear equations, so

1. **An Iterative method is required.**
2. **Very good estimate of initial guess is required.**
3. **No guarantee of finding a solution.**

01 Tasks Update - W_{max} Solution

Solution:

- **MINPACK (Garbow et al., 1980) *HYBRID* method is able to provide a solution.**
- **Other iterative methods (*Levenberg-Marquardt*, *Broyden*, *Newton-Krylov* etc.) is not stable.**
- **$L_{max}/2$ and $2W$ are good starting values (but not optimum)**

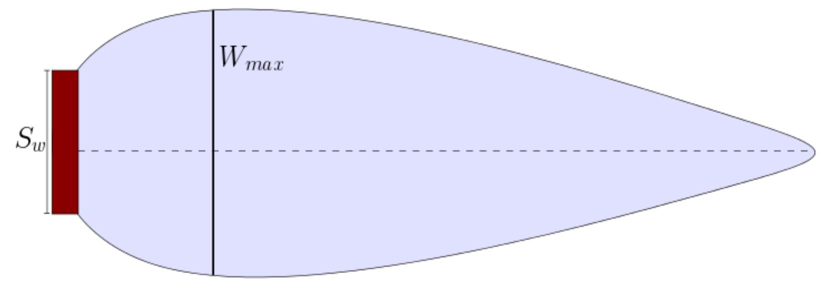
Works to be done:

1. **Find a more optimum starting values so that a unique solution is guaranteed.**
2. **Re-evaluate the problem statement by considering several terms of the infinite series that is available in the given equation for *C***

01 Tasks Update - W_{max} Solution

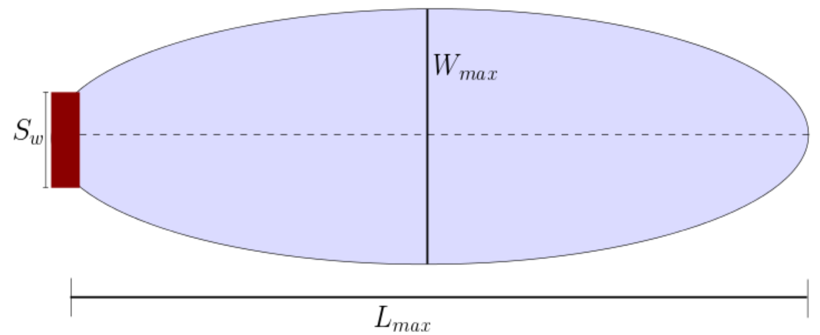
Initial result analysis for W_{max}

- Larger Source Width (S_w) results to W_{max} closer to the source



- Horizontal Transverse dispersivity (α_{Th}) affects the magnitude of W_{max}.

Outlook:



- It is possible to estimate:
  - ✓ $A_{max} = L_{max} \times W_{max}$
  - ✓ $V_{max} = A_{max} \times M$, with M = aquifer thickness
- Remidiation cost can be estimated.