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A THERMODYNAMICALLY CONSISTENT MODEL FOR TURBULENT, BINARY MIXTURE UNDERGOING PHASE TRANSITION

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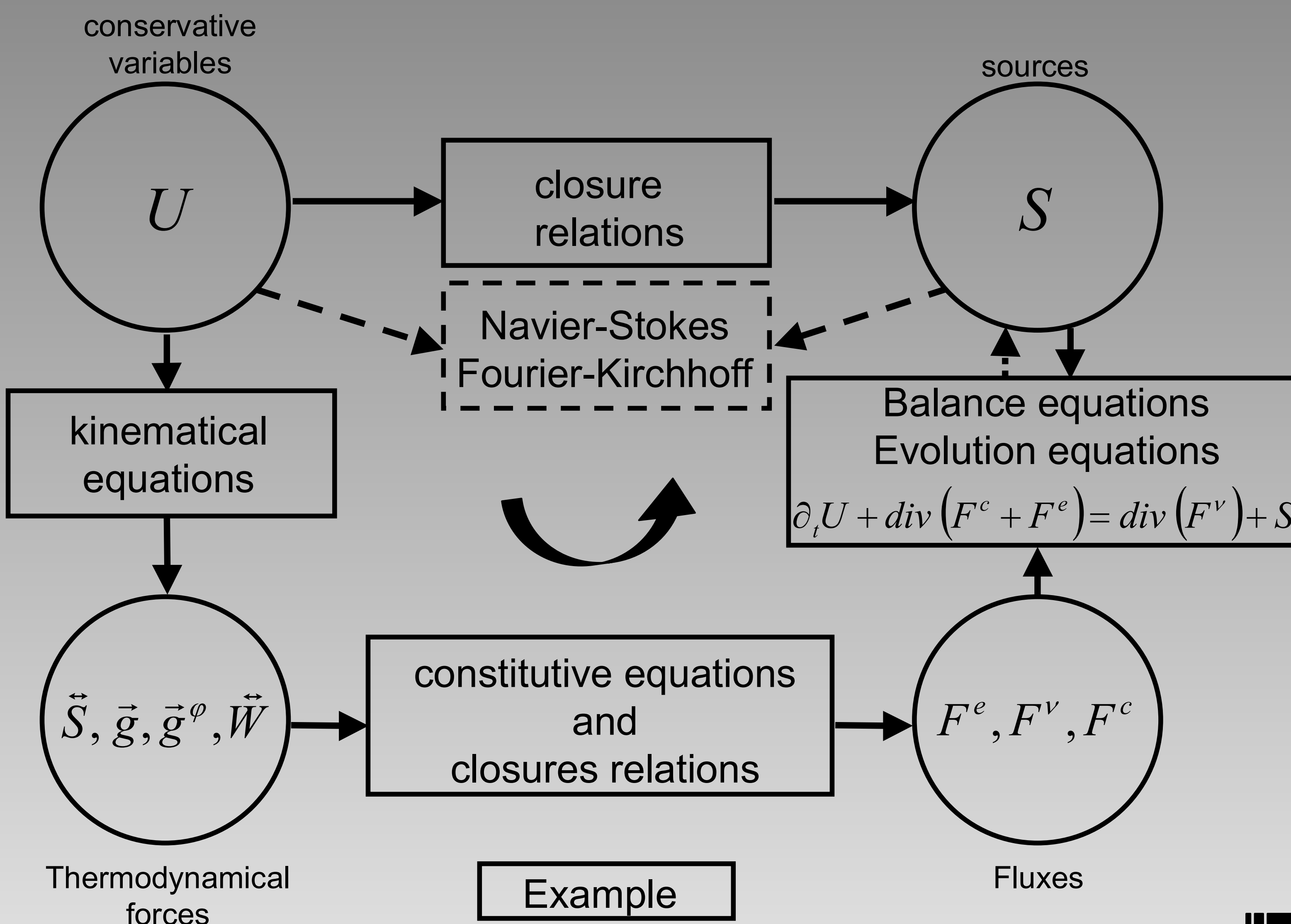
Three-stages organization of CFD commercial codes.

The basic denotations



Example

$$U \equiv \left\{ \begin{array}{c} \rho \\ \rho\vec{v} \\ \rho e \\ - - - \\ \rho k \\ \rho\varepsilon \\ - - - \\ \rho Y_{(k)} \\ - - - \\ \rho\alpha \\ \rho\alpha_{ij} \end{array} \right\}$$

balance equations

evolution equations

deformation rate

$$\overleftrightarrow{S} = \frac{1}{2}\left(grad\ \vec{v} + grad^T\ \vec{v}\right) = S_{ij}\ \vec{e}_i \otimes \vec{e}_j$$

vorticity

$$\overleftrightarrow{W} = \frac{1}{2}\left(grad\ \vec{v} - grad^T\ \vec{v}\right) = W_{ij}\ \vec{e}_i \otimes \vec{e}_j$$

gradient of temperature

$$\vec{g} = \nabla T = grad\ T = g_i\ \vec{e}_i$$

gradient of scalar φ

$$\vec{g}^{\varphi} = \nabla\varphi = grad\ \varphi = g_i^{\varphi}\ \vec{e}_i$$

viscous flux of momentum

wrong $$\tau_{ij} = \mu\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) - \frac{1}{3}\frac{\partial v_k}{\partial x_k}\delta_{ij}$$

correct $$\tau_{ij} = 2\mu\, S_{ij} - \frac{2}{3}\mu\, I_s \delta_{ij} + \mu_2\, S_{ik}\, S_{kj}$$

$$I_s = tr\,\overleftrightarrow{S}$$

$$II_s = adj\,\overleftrightarrow{S}$$

$$III_s = \det\,\overleftrightarrow{S}$$

balance of momentum

curvilinear coordinate system

$$\partial_t\left(\rho\,\vec{v}\right)+div\left(\rho\,\vec{v}\otimes\vec{v}+\overleftrightarrow{p}\right)=div\left(\overleftrightarrow{\tau}+\overleftrightarrow{R}+\overleftrightarrow{\tau}^{D}+....\right)+\rho\,\overleftrightarrow{b}$$

Cartesian coordinate system i, j=x, y, z

$$\frac{\partial}{\partial t}\left(\rho\,v_i\right)+\frac{\partial}{\partial x_j}\left(\rho\,v_i\,v_j+p\,\delta_{ij}\right)=\frac{\partial}{\partial x_j}\left(\tau_{ij}+R_{ij}+\tau_{ij}{}^{D}+....\right)+\rho\,b_i$$

scalar evolution equation

present: $$\frac{\partial}{\partial t}\rho\varphi + \frac{\partial}{\partial x_i}\left(\rho\varphi v_i\right) = \frac{\partial}{\partial x_i}\left(D_p \frac{\partial}{\partial x_i}\varphi\right) + \rho S_\varphi$$

correctly should be:

evolution equation

$$\frac{\partial}{\partial t}\left(\rho\, v_i\right) + \frac{\partial}{\partial x_i}\left(\rho\ \varphi\ v_i\right) = \frac{\partial}{\partial x_i} T_i^\varphi + \rho\ S_\varphi$$

closure equations

$$T_i^\varphi = D_\varphi g_i^\varphi$$

or

$$T_i^\varphi = D_{ij}^\varphi g_j^\varphi + D^T g_i + D^k g_i^k$$

kinematical equations

$$g_i^\varphi = \frac{\partial}{\partial x_i}\varphi \ , \quad g_i = \frac{\partial}{\partial x_i} T \quad , \quad g_i^k = \frac{\partial}{\partial x_i} k$$

Extension of the Reynolds splitting procedure

	two – scalar equations	Scalar – symmetric tensor equations	other models
Turbulent mass microstructure	$k_\rho = \left(\rho'\rho'\right)''$ $\varepsilon_\rho = \left(\rho',_i \rho',_i\right)''$	$k_\rho = \left(\rho'\rho'\right)''$ $\varepsilon_{ij}^{\rho} = \left(\rho',_i \rho',_j\right)''$	$\varepsilon_{ij}^{\rho} = \left(\rho'\rho',_i\right)''$
Turbulent momentum microstructure	$2k = \left(\rho' v_i' v_i'\right)''$ $\varepsilon = \left(\rho' v_{i,j} v_{i,j}\right)''$	$k_{ij} = \left(\rho' v_i' v_j'\right)''$ $\varepsilon_{ij} = \left(\rho' v_{i,k} v_{i,k}\right)''$	$k = \left(\rho' v_i' v_i'\right)''$ and 9 – component $\lambda_{ij} = \left(\rho' v_i',_j\right)''$
Turbulent energy microstructure	$k_\theta = \left(\rho' T' T'\right)''$ $\varepsilon_\theta = \left(\rho' T',_i T',_i\right)''$	$k_\theta = \left(\rho' T' T'\right)''$ $\varepsilon_{ij}^{\theta} = \left(\rho' T',_i T',_j\right)''$	$\varepsilon_i^{\theta} = \left(\rho' T,_j\right)''$

Consistent Thermodynamics of Water-Air Turbulent Mixture

The set of internal parameters

21 internal parameters $\left\{\varphi, k, \varepsilon, \varphi_{ij}, J_{ij}^{t}, \varepsilon_{ij}\right\}, \quad i, j = x, y, z$

$$\alpha = \left\{\varphi, k, \varepsilon\right\} \ ,$$

$$\alpha_{ij} = \left\{\varphi_{ij}, J_{ij}^{t}, \varepsilon_{ij}\right\}.$$

three macroscopic unknowns,

$$\rho, \mathbf{v}, T$$

Internal energy

extended Gibbs :

$$d\,u = \frac{\partial u}{\partial \rho}\Big|_{s,\alpha,\alpha_{ij}} d\rho + \frac{\partial u}{\partial \rho}\Big|_{s,\alpha,\alpha_{ij}} ds + \frac{\partial u}{\partial \rho}\Big|_{s,\alpha,\alpha_{ij}} d\alpha + \frac{\partial u}{\partial \rho}\Big|_{s,\alpha,\alpha_{ij}} d\alpha_{ij} =$$

$$= \mu\, d\rho + T ds + A^{(r)} d\alpha + A_{ij}{}^{(r)} d\alpha_{ij}$$

$A^{(r)} \equiv A$ and $A_{ij}{}^{(r)} \equiv A_{ij}$

$\alpha_{ij}^{0} = k_0 \sigma_0 r_0^2 \delta_{ij}$ (r_0 - radius of bubble), :

$$u = u_{\alpha}(\rho, s, \alpha) + \alpha \left[k_0 \frac{\sigma}{\sigma_0} r_0^3 \left(\frac{3\alpha_{ij}}{k_0 r_0^2} - \delta_{ij} \right)^2 \right]$$

where $\sigma_0(r_0)$ - surface tension.

$$A_{ij} = A_{ji} = \alpha\, K \left(\frac{3\alpha_{ij}}{k_0 r_0^2} - \delta_{ij} \right)$$

Total energy.

$$e = u + 0.5\mathbf{v} \cdot \mathbf{v}$$

The vector of unknowns conservative variables

$$U = \left\{\rho, \mathbf{v}, e, \rho\,\alpha, \rho\,\alpha_{ij}\right\}$$

Evolution equations

so-called "conservative form" :

$$\partial_t U + \operatorname{div}\left(F^c + F^e\right) = \operatorname{div}\left(F^v\right) + S$$

In our case the equations of balance take on the following local form:

Balance of mass

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}\left(\rho v_i\right) = 0$$

Balance of momentum

$$\frac{\partial}{\partial t}\left(\rho v_i\right) + \frac{\partial}{\partial x_j}\left(\rho v_i v_j + p_{ij}\right) = \frac{\partial}{\partial x_j}\left(\tau^c{}_{ij}\right) + \rho b_i$$

Balance of energy

$$\frac{\partial}{\partial t}\left(\rho\, e\right) + \frac{\partial}{\partial x_j}\left(\rho\, e v_j + p_{jk} v_k + p_i^\alpha A + p_{jik}^\alpha A_{ik}\right) =$$

$$= \frac{\partial}{\partial x_j}\left(q_j^c + \tau^c{}_{ij} v_i + J_j^\alpha A + J_{jik}^\alpha A_{ik}\right) + \rho\, b_i v_i + \rho\left(A^{(tot)} s^\alpha + A_{ij}{}^{(tot)} s_{ij}^\alpha\right)$$

Evolution of the scalar microstructure $\alpha = \{\varphi, k, \varepsilon\}$

$$\frac{\partial}{\partial t}(\rho\alpha) + \frac{\partial}{\partial x_j}\left(\rho\alpha v_j + p_j^{\alpha}\right) = \frac{\partial}{\partial x_j}\left(J_j^{\alpha}\right) + \rho s^{\alpha}$$

Evolution of the tensor microstructure $\alpha_{ij} = \{\varphi_{ij}, J_{ij}^{t}, \varepsilon_{ij}\}$

$$\frac{\partial}{\partial t}(\rho\alpha_{ij}) + \frac{\partial}{\partial x_k}\left(\rho\alpha_{ij} v_k + p_{ijk}^{\alpha}\right) = \frac{\partial}{\partial x_k}\left(J_{ijk}^{\alpha}\right) + \rho s_{ij}{}^{\alpha}$$

the total dissipative momentum flux $\tau^c{}_{ij}$ is the sum of the molecular, operative, turbulent and diffusive fluxes:

$$\tau^c{}_{ij} = \tau_{ij} + J_{ij}^{op} + J_{ij}^{t} + J_{ij}^{d} \ ,$$

and the total dissipative energy flux:

$$q_j^c = TJ_i^s + J_i^{op} + J_i^{t} + J_i^{d}$$

Clausius-Duhem

evolution equation for the entropy micro-sub-structure

$$\rho \frac{d}{dt} s \equiv \rho \dot{s} = \frac{\partial}{\partial t}(\rho s) + \frac{\partial}{\partial x_j}\left(\rho s v_j\right) = \frac{\partial}{\partial x_j}\left(J_j^s\right) + \rho \sigma_s \ ,$$

where, according to the Second Law of Thermodynamics :

$$\sigma_s \geq 0 \, .$$

Irreversible properties of continua.

the expression for $\dot{e}$:

$$\rho\,\dot{e} = \rho\,\dot{u} + \rho\,v_i\dot{v}_i = \rho\left(\mu\dot{\rho} + T\dot{s} + A\dot{\alpha} + A_{ij}\dot{\alpha}_{ij} + v_i\dot{v}_i\right)$$

$\mu\dot{\rho},\ T\dot{s},\ A\dot{\alpha},\ A_{ij}\alpha_{ij},\ v_i\dot{v}$ - by multiplication of :

balance of mass by $\mu\dot{\rho}$

$$\mu\rho\left(\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}\left(\rho v_i\right)\right) = \mu\rho\left(\dot{\rho} + \rho\frac{\partial}{\partial x_i}\left(v_i\right)\right) = 0$$

balance of momentum by v_i

$$\rho\,v_i\left(\dot{v}_i\right) + v_i\frac{\partial}{\partial x_j}\left(p_{ij}\right) = v_i\frac{\partial}{\partial x_j}\left(\tau^c{}_{ij}\right) + \rho\,v_i b_i$$

balance of scalar microstructure by A

$$\rho A(\dot{\alpha}) + A\frac{\partial}{\partial x_j}\left(p_j^{\alpha}\right) = A\frac{\partial}{\partial x_j}\left(J_j^{\alpha}\right) + \rho A s^{\alpha}$$

balance of tensor microstructure by A_{ij}

$$\rho A_{ij}\left(\dot{\alpha}_{ij}\right) + A_{ij}\frac{\partial}{\partial x_k}\left(p_{ijk}^{\alpha}\right) = A_{ij}\frac{\partial}{\partial x_k}\left(J_{ijk}^{\alpha}\right) + \rho A_{ij} s_{ij}{}^{\alpha}$$

balance of the specific entropy by T

$$\rho T\dot{s} = T\frac{\partial}{\partial x_j}\left(J_j^{s}\right) + \rho T\sigma_s$$

$\rho\dot{e}$ also can be expressed from the balance of energy as

$$\rho\dot{e}+\frac{\partial}{\partial x_j}\left(p_{jk}v_k+p_i^{\alpha}A+p_{jik}^{\alpha}A_{ik}\right)=$$

$$=\frac{\partial}{\partial x_j}\left(TJ_j^s+\tau^c{}_{ij}v_i+J_j^{\alpha}A+J_{jik}^{\alpha}A_{ik}\right)+\rho b_i v_i+\rho\left(A^{(tot)}s^{\alpha}+A_{ij}{}^{(tot)}s_{ij}^{\alpha}\right)$$

Now, making the difference between energy balances and substituting additionally a few identity of the following type :

$$\frac{\partial}{\partial x_i}\left(\tau_{ij}^c v_j\right)=v_j\frac{\partial}{\partial x_i}\left(\tau_{ji}^c\right)+\tau_{ij}^c\frac{\partial}{\partial x_i}v_j$$

we obtain as a result the following relation for entropy production:

$$\rho T\sigma_s=\tau_{ij}^c\left(v_{i,j}\right)+J_j^sT_{,j}+J_j^aA_{,j}+J_{jik}^{\alpha}A_{ik,j}+$$
$$+\rho\left(A^{(tot)}-A\right)s^{\alpha}+\rho\left(A_{ij}{}^{(tot)}-A_{ij}\right)s_{ij}^{\alpha}$$

The associated dissipation functional is $2D=T\sigma_s$

Onsager-Casimir relations

$$D = J \circ X$$

where J are thermodynamical fluxes

X are thermodynamical forces.

$$J = \left\{ \tau_{ij}^{c}, J_{i}^{c}, J_{i}^{\alpha}, J_{ijk}^{\alpha}, \rho s^{a}, \rho s_{ij}^{\alpha} \right\} ,$$

$$X = \left\{ v_{i,j}, T_{,i}, A_{,i}\ A_{ij,k}, A^{(tot)} - A, A_{ij}^{(tot)} - A_{ij} \right\} .$$

the linear case : $J_a = L_{ab} X_b$

- total dissipative momentum flux

$$\tau_{ij}^c = L_{11}(\varphi, k, \varepsilon)\, d_{ij} + L_{16}\left(A_{ij}{}^{(tot)} - A_{ij}\right) + \left[L_{17} v_{i,i} + L_{15}\left(A^{(tot)} - A\right)\right]\delta_{ij}$$

- the entropy flux

$$J_i^c = T q_i^c = L_{22} T_{,i} + L_{23} A_{,i}$$

- the flux of scalar microstructure $\alpha = \{\varphi, k, \varepsilon\}$

$$J_i^\alpha = L_{32} T_{,i} + L_{33} A_{,i}$$

- the flux of tensorial microstructure $\alpha_{ij} = \left\{\varphi_{ij}, J^t_{ij}, \varepsilon_{ij}\right\}$

$$J^{\alpha}_{ijk} = L_{14} d_{ij},_k + L_{44} A_{ij},_k$$

- the scalar source $\alpha = \left\{\varphi, k, \varepsilon\right\}$

$$\rho s^{\alpha} = L_{15}(\varphi, k, \varepsilon)\, d_{ii} + L_{45}\left(A_{ii}{}^{(tot)} - A_{ii}\right) + L_{35}\left(A^{(tot)} - A\right)$$

- the tensorial source $\alpha_{ij} = \left\{\varphi_{ij}, J^t_{ij}, \varepsilon_{ij}\right\}$

$$\rho s_{ij}{}^{\alpha} = L_{16}(\varphi, k, \varepsilon)\, d_{ij} + L_{66}\left(A_{ij}{}^{(tot)} - A_{ij}\right) + L_{63}\left(A^{(tot)} - A\right)\delta_{ij}$$

Turbulent evolution of the water-air structure

the internal variables

$$\alpha = \{\varphi, k, \varepsilon\}$$

$$\alpha_{ij} = \{\varphi_{ij}, 0, 0\}.$$

$$\rho\dot{\varphi} = \frac{\partial}{\partial x_i}\left(J_i^{\varphi}\right) \, ,$$

$$\rho\dot{\varphi}_{ij} = \rho s_{ij}^{\varphi} \quad .$$

three scalar affinity A^{φ}, A^{k}, A^{ε} and one tensor A_{ij}^{φ} should be defined.

$$\tau_{ij}^{c} = 2\left(\mu + \mu_{t} + \mu_{op}\right) d_{ij} + \lambda^{op} v_{i},_{i} \delta_{ij} + \mu_{1}\left(A_{ij}{}^{tot} - A_{ij}^{\varphi}\right) + \\ + \left[\mu_{2}\left(A_{k}^{tot} - A^{k}\right) + \mu_{2}\left(A_{\varphi}^{tot} - A^{\varphi}\right)\right]\delta_{ij}$$

$$J_{i}^{c} = Tq_{i}^{c} = \left(\lambda + \lambda^{t}\right) T,_{i} + \lambda_{1} A^{\varphi},_{i} + \lambda_{2} A^{k},_{i} + \lambda_{3} A^{\varepsilon},_{i}$$

$$J_{i}^{\varphi} = \left(\kappa + \kappa^{t}\right) T,_{i} + \kappa_{1} A^{\varphi},_{i} + \kappa_{2} A^{k},_{i} + \kappa_{3} A^{\varepsilon},_{i}$$

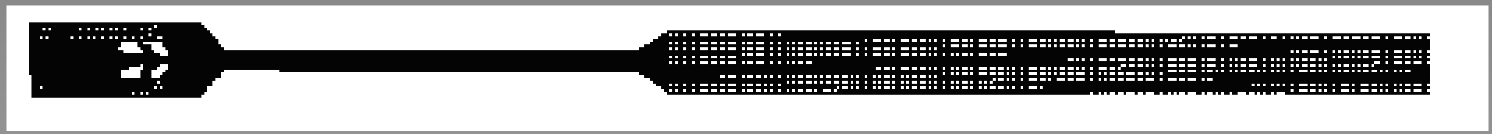
$$\rho s_{ij}^{\varphi} = \beta_{1}\left(A_{ij}{}^{tot} - A_{ij}^{\varphi}\right) + \beta_{2} d_{ij} + \left[\beta_{3}\left(A_{k}^{tot} - A^{k}\right) + \beta_{4}\left(A_{\varphi}^{tot} - A^{\varphi}\right)\right]\delta_{ij}$$

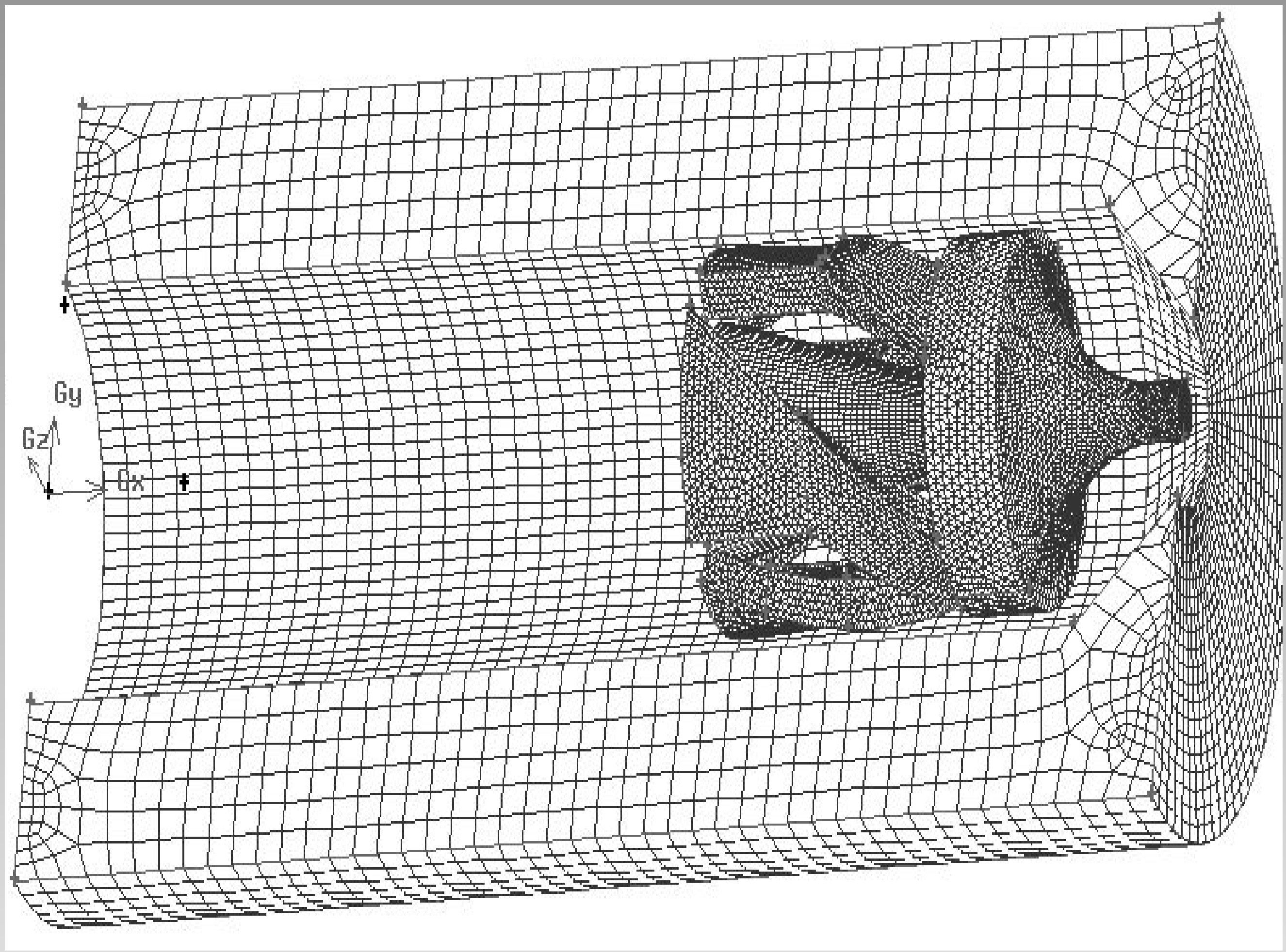
where appears a numerous coefficients :

$$\mu, \mu^{t}, \mu^{op}, \mu_{1}, \mu_{2}, \mu_{3}, \lambda, \lambda^{op}, \lambda^{t}, \kappa, \kappa^{t}, \ldots, \beta_{4}$$

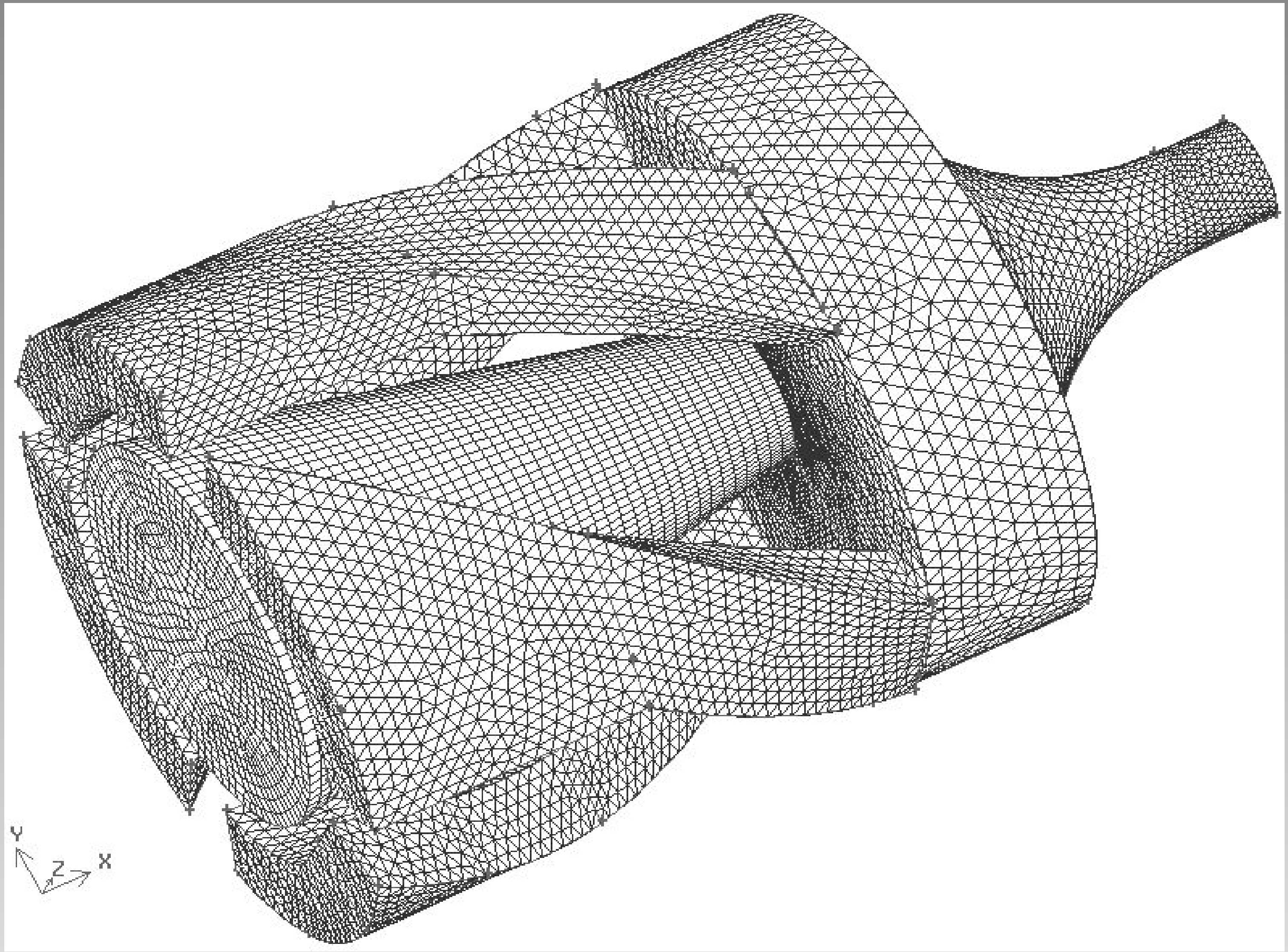
that, in generally can be the functions of $\left\{\varphi, k, \varepsilon, \varphi_{ij}\right\}$

WATER-AIR TURBULENT MIXTURE FLOW WITHIN AN EJECTOR



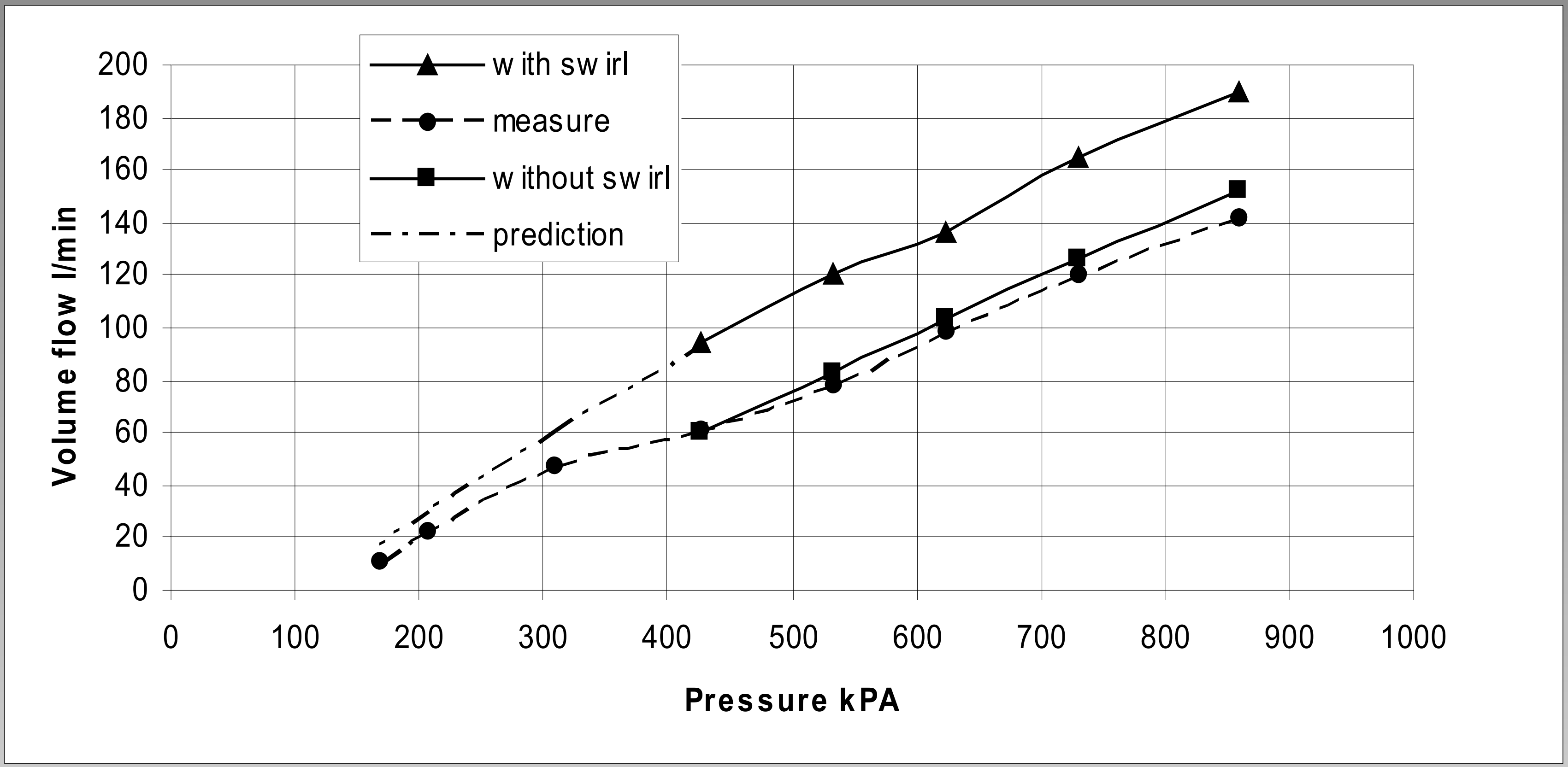


GEOMETRY OF THE SWIRL

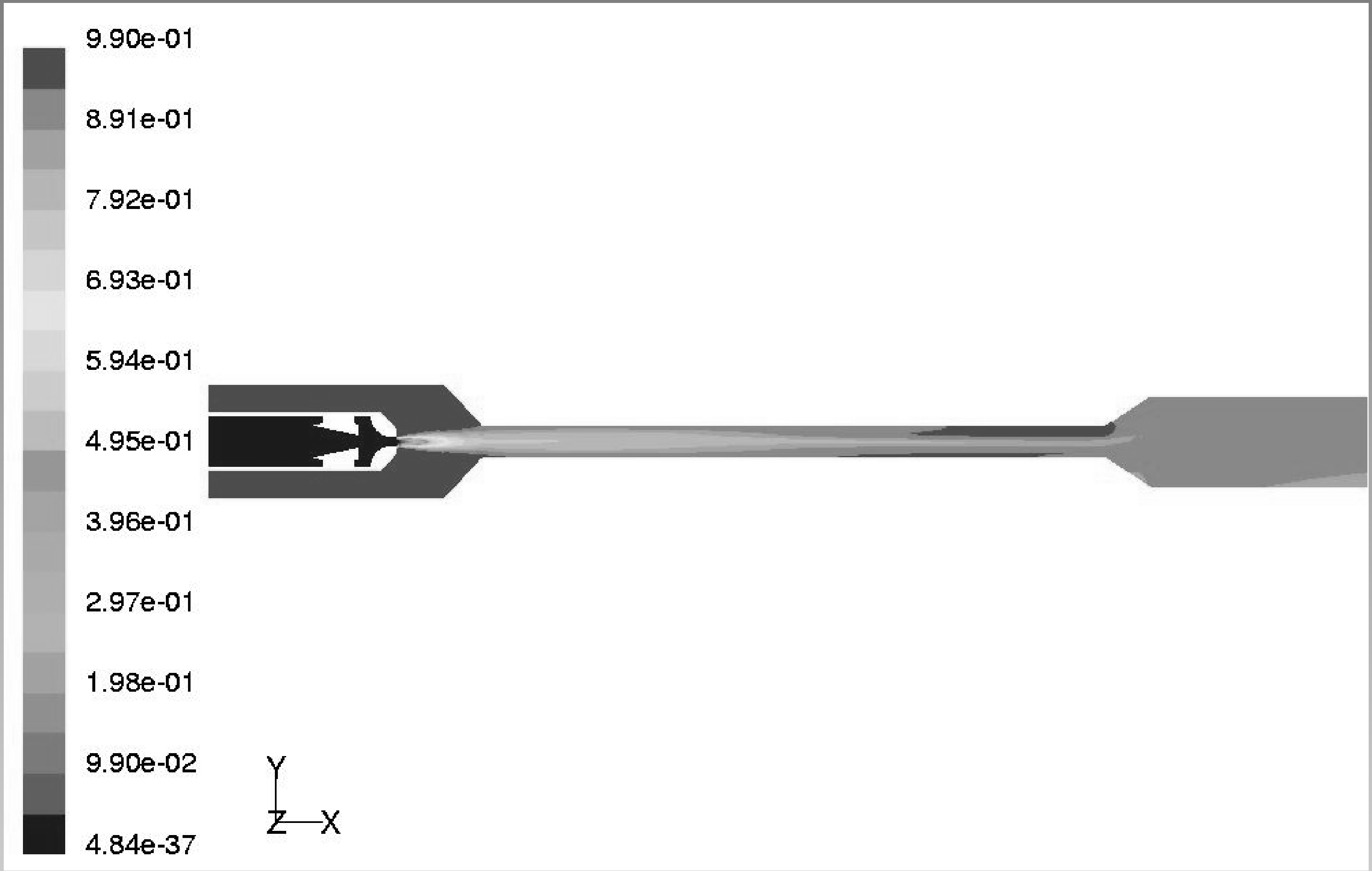


Comparison of calculated and measured volumetric flows

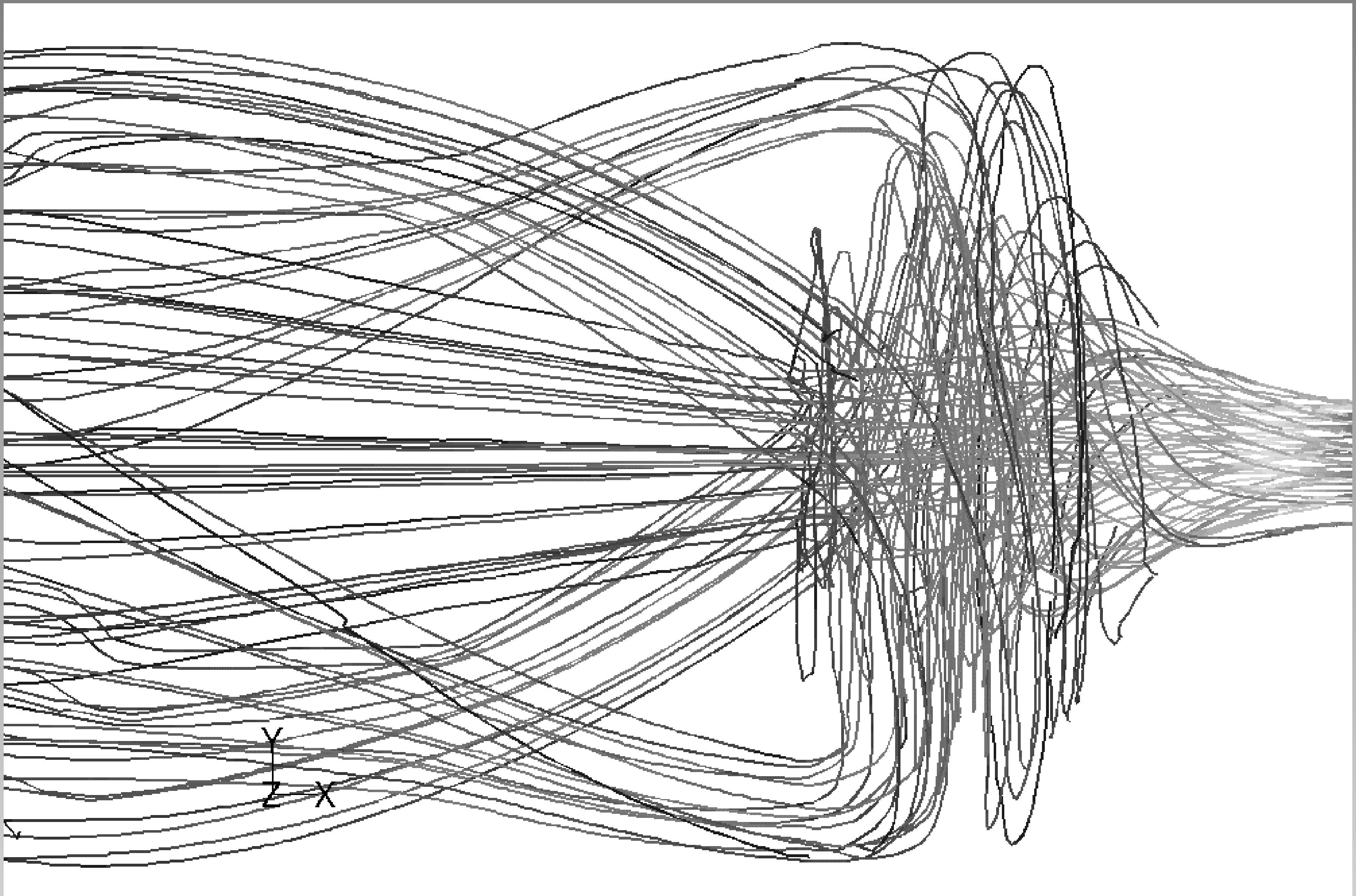
RUN	Measured		Simulations without swirl		Simulations with swirl		
	water	air	water	air	water	Air	
	l/min	l/min	l/min	l/min	l/min	l/min	
701	21,51	141,5	20,043	141,26	18,52535	190,0796	0,34
702	19,91	120,1	18,38448	117,155	17,05871	164,2489	0,37
703	17,91	98,59	16,88508	96,475	15,556	136,7337	0,39
704	16,24	78,84	15,42852	77,689	14,91284	120,1685	0,53
705	14,11	61,1	13,53744	55,597	12,37628	94,33786	0,54
706	11,33	48,06	11,01233	31,036	-	-	-
707	8,05	23,22	7,947432	-	-	-	-
708	6,45	11,44	6,6402	-	-	-	-



w ith sw irl
measure
w ithout sw irl
prediction
Volume flow l/min
Pressure kPA
0
20
40
60
80
100
120
140
160
180
200
0
100
200
300
400
500
600
700
800
900
1000



Volume fraction of air



flow lines within the swirl