Project Mathematical Engineering

Group 1
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1 Theoretical computations

1.1 Initial system of equations

We start with the initial non–linear reaction–diffusion equations in a stationary regime for $(r, z) \in \Omega$:

$$\begin{cases} \nabla \cdot \left(r \begin{pmatrix} \sigma_{u,r} & 0 \\ 0 & \sigma_{u,z} \end{pmatrix} \nabla C_u(r,z) \right) = rR_u(C_u(r,z), C_v(r,z)) \\ \nabla \cdot \left(r \begin{pmatrix} \sigma_{v,r} & 0 \\ 0 & \sigma_{v,z} \end{pmatrix} \nabla C_v(r,z) \right) = -rR_v(C_u(r,z), C_v(r,z)) \end{cases}$$

We continue only with the equation for oxygen and subscript u, seeing that the case for carbon dioxide and subscript v is similar. We write

$$\begin{cases} \vec{q}_u(r,z) = r \begin{pmatrix} \sigma_{u,r} & 0 \\ 0 & \sigma_{u,z} \end{pmatrix} \nabla C_u(r,z) \\ \vec{q}_v(r,z) = r \begin{pmatrix} \sigma_{v,r} & 0 \\ 0 & \sigma_{v,z} \end{pmatrix} \nabla C_v(r,z) \end{cases}$$

such that

$$\begin{cases} \nabla \cdot \vec{q}_u(r,z) = rR_u(C_u(r,z), C_v(r,z)) \\ \nabla \cdot \vec{q}_v(r,z) = -rR_v(C_u(r,z), C_v(r,z)) \end{cases}$$

Similarly, the boundary conditions for $(r, z) \in \Gamma$ are the following:

$$\begin{cases} -\vec{n}(r,z) \cdot \left(\begin{pmatrix} \sigma_{u,r} & 0 \\ 0 & \sigma_{u,z} \end{pmatrix} \nabla C_u(r,z) \right) & = \rho_u C_u^*(r,z) \\ -\vec{n}(r,z) \cdot \left(\begin{pmatrix} \sigma_{v,r} & 0 \\ 0 & \sigma_{v,z} \end{pmatrix} \nabla C_v(r,z) \right) & = \rho_v C_v^*(r,z) \end{cases}$$

and become

$$\begin{cases} -\vec{n}(r,z) \cdot \vec{q}_u(r,z) = r\rho_u C_u^*(r,z) \\ -\vec{n}(r,z) \cdot \vec{q}_v(r,z) = r\rho_v C_v^*(r,z) \end{cases}$$

Now using linear basis functions $\varphi_i(r,z)$, we define the weak formulations as (integrating on Ω):

$$\begin{cases} \int_\Omega (\nabla \cdot \vec{q}_u(r,z))\varphi(r,z)d\Omega = \int_\Omega rR_u(C_u(r,z), C_v(r,z))\varphi(r,z)d\Omega \\ \int_\Omega (\nabla \cdot \vec{q}_v(r,z))\varphi(r,z)d\Omega = -\int_\Omega rR_v(C_u(r,z), C_v(r,z))\varphi(r,z)d\Omega \end{cases}$$

$$\begin{cases} \int_\Gamma (-\vec{n}(r,z) \cdot \vec{q}_u(r,z))\varphi(r,z)d\Gamma = \int_\Gamma r\rho_u C_u^*(r,z)\varphi(r,z)d\Gamma \\ \int_\Gamma (-\vec{n}(r,z) \cdot \vec{q}_v(r,z))\varphi(r,z)d\Gamma = \int_\Gamma r\rho_v C_v^*(r,z)\varphi(r,z)d\Gamma \end{cases}$$

Furthermore, the divergence theorem teaches us that

$$\begin{cases} \int_\Omega (\nabla \cdot \vec{q}_u(r,z))\varphi(r,z)d\Omega = -\int_\Omega \vec{q}_u(r,z) \cdot \nabla\varphi(r,z)d\Omega + \int_\Gamma (\vec{n}(r,z) \cdot \vec{q}_u(r,z))\varphi(r,z)d\Gamma \\ \int_\Omega (\nabla \cdot \vec{q}_v(r,z))\varphi(r,z)d\Omega = -\int_\Omega \vec{q}_v(r,z) \cdot \nabla\varphi(r,z)d\Omega + \int_\Gamma (\vec{n}(r,z) \cdot \vec{q}_v(r,z))\varphi(r,z)d\Gamma \end{cases}$$

so that the weak formulations become

$$\begin{cases} \int_\Omega \vec{q}_u(r,z) \cdot \nabla\varphi(r,z)d\Omega + \int_\Omega rR_u(C_u, C_v)\varphi(r,z)d\Omega + \int_\Gamma r\rho_u C_u^*(r,z)\varphi(r,z)d\Gamma = 0 \\ \int_\Omega \vec{q}_v(r,z) \cdot \nabla\varphi(r,z)d\Omega - \int_\Omega rR_v(C_u, C_v)\varphi(r,z)d\Omega + \int_\Gamma r\rho_v C_v^*(r,z)\varphi(r,z)d\Gamma = 0 \end{cases} \tag{1}$$

Using the triangulation with M vertices, we make use of the fact that

$$\begin{cases} C_u(r,z) \approx C_u^M(r,z) \equiv \sum_{i=1}^{M} c_i\varphi_i(r,z) \\ C_v(r,z) \approx C_v^M(r,z) \equiv \sum_{i=1}^{M} c_{M+i}\varphi_i(r,z) \end{cases}$$

with a coefficient vector $c = (c_u, c_v) \in \mathbb{R}^{2M}$ to retrieve a system of linear equations. We can then rewrite (1) in a parametric form as

$$\begin{pmatrix} K_u & 0 \\ 0 & K_v \end{pmatrix} \begin{pmatrix} c_u \\ c_v \end{pmatrix} - \begin{pmatrix} f_u \\ f_v \end{pmatrix} + \begin{pmatrix} H_u(c_u, c_v) \\ H_v(c_u, c_v) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{2}$$

1.2 First part of system (2)

Making use of the triangulation, we can write that

$$\begin{cases} \displaystyle\int_\Omega \vec{q}_u(r,z)\cdot\nabla\varphi(r,z)d\Omega \approx \begin{pmatrix}\sigma_{u,r} & 0\\ 0 & \sigma_{u,z}\end{pmatrix}\sum_{i=1}^{M} c_i \int_\Omega r\nabla\varphi_i(r,z)\cdot\nabla\varphi(r,z)d\Omega \\ \displaystyle\int_\Omega \vec{q}_v(r,z)\cdot\nabla\varphi(r,z)d\Omega \approx \begin{pmatrix}\sigma_{v,r} & 0\\ 0 & \sigma_{v,z}\end{pmatrix}\sum_{i=1}^{M} c_{M+i} \int_\Omega r\nabla\varphi_i(r,z)\cdot\nabla\varphi(r,z)d\Omega \end{cases}$$

which reduces to

$$\begin{cases} \displaystyle\int_\Omega \vec{q}_u(r,z)\cdot\nabla\varphi(r,z)d\Omega \approx \begin{pmatrix}\sigma_{u,r} & 0\\ 0 & \sigma_{u,z}\end{pmatrix}\sum_{i=1}^{M} c_i a_i \equiv K_u c_u \\ \displaystyle\int_\Omega \vec{q}_v(r,z)\cdot\nabla\varphi(r,z)d\Omega \approx \begin{pmatrix}\sigma_{v,r} & 0\\ 0 & \sigma_{v,z}\end{pmatrix}\sum_{i=1}^{M} c_{M+i} a_i \equiv K_v c_v \end{cases}$$

provided the introduction of a variable

$$\begin{aligned} a_i &= \int_\Omega r\nabla\varphi_i(r,z)\cdot\nabla\varphi(r,z)d\Omega \\ &= \sum_{j\in\mathcal{J}_i}\int_{\Omega_j} r\nabla\varphi_i(r,z)\cdot\nabla\varphi(r,z)d\Omega \end{aligned}$$

with $\mathcal{J}_i$ the set of all j such that the basis functions $\varphi_i(r,z)$ are non-zero inside Ω_j.

1.2.1 Change of coordinates

Introducing a new coordinate system (ξ,η), we define in the triangle Ω_j composed of three points $(r_1,z_1),(r_2,z_2),(r_3,z_3)$:

$$\begin{aligned} \xi &= \frac{1}{2|\Omega_j|}((z_3-z_1)(r-r_1)-(r_3-r_1)(z-z_1)) \\ \eta &= \frac{1}{2|\Omega_j|}(-(z_2-z_1)(r-r_1)+(r_2-r_1)(z-z_1)) \end{aligned}$$

with basis functions in that coordinate system

$$\begin{aligned} \psi_1(\xi,\eta) &= 1-\xi-\eta \\ \psi_2(\xi,\eta) &= \xi \\ \psi_3(\xi,\eta) &= \eta \end{aligned}$$

and $|\Omega_j|$ the area of the triangle, given in the (r,z) plane by

$$2|\Omega_j| = \begin{vmatrix}1 & r_1 & z_1\\ 1 & r_2 & z_2\\ 1 & r_3 & z_3\end{vmatrix} = \begin{vmatrix} r_2-r_1 & z_2-z_1\\ r_3-r_1 & z_3-z_1\end{vmatrix}$$

We can then retrieve

$$r = r_1 + (r_2 - r_1)\xi + (r_3 - r_1)\eta$$
$$z = z_1 + (z_2 - z_1)\xi + (z_3 - z_1)\eta$$

Our integration constant can also be changed in the following way:

$$d\Omega = \begin{vmatrix} \frac{\partial r}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial r}{\partial \eta} & \frac{\partial z}{\partial \eta} \end{vmatrix} d\xi d\eta = \begin{vmatrix} r_2 - r_1 & z_2 - z_1 \\ r_3 - r_1 & z_3 - z_1 \end{vmatrix} d\xi d\eta = 2|\Omega_j| d\xi d\eta$$

so that integrating on the triangle Ω_j is equivalent to integrating η from 0 to $1-\xi$ and then ξ from 0 to 1.

Furthermore, the differentiation of the basis functions φ_i that are non-zero inside Ω_j, that will also be used as test functions φ, becomes

$$\begin{bmatrix} \frac{\partial}{\partial r}\psi_1(\xi,\eta) & \frac{\partial}{\partial z}\psi_1(\xi,\eta) \\ \frac{\partial}{\partial r}\psi_2(\xi,\eta) & \frac{\partial}{\partial z}\psi_2(\xi,\eta) \\ \frac{\partial}{\partial r}\psi_3(\xi,\eta) & \frac{\partial}{\partial z}\psi_3(\xi,\eta) \end{bmatrix} = \frac{1}{2|\Omega_j|} \begin{bmatrix} z_2 - z_3 & r_3 - r_2 \\ z_3 - z_1 & r_1 - r_3 \\ z_1 - z_2 & r_2 - r_1 \end{bmatrix}$$

1.2.2 Final parametrization

With the change of coordinates, our a_i become the following:

$$\begin{aligned} a_i &= \int_0^1 \int_0^{1-\xi} r \frac{1}{4|\Omega_j|^2} \begin{bmatrix} z_2 - z_3 & r_3 - r_2 \\ z_3 - z_1 & r_1 - r_3 \\ z_1 - z_2 & r_2 - r_1 \end{bmatrix} \begin{bmatrix} z_2 - z_3 & r_3 - r_2 \\ z_3 - z_1 & r_1 - r_3 \\ z_1 - z_2 & r_2 - r_1 \end{bmatrix}^T 2|\Omega_j| d\eta d\xi \\ &= \frac{1}{2|\Omega_j|} \begin{bmatrix} z_2 - z_3 & r_3 - r_2 \\ z_3 - z_1 & r_1 - r_3 \\ z_1 - z_2 & r_2 - r_1 \end{bmatrix} \begin{bmatrix} z_2 - z_3 & z_3 - z_1 & z_1 - z_2 \\ r_3 - r_2 & r_1 - r_3 & r_2 - r_1 \end{bmatrix} \int_0^1 \int_0^{1-\xi} r d\eta d\xi \end{aligned}$$

where

$$\begin{aligned} \int_0^1 \int_0^{1-\xi} r d\eta d\xi &= \int_0^1 \int_0^{1-\xi} (r_1 + (r_2 - r_1)\xi + (r_3 - r_1)\eta) d\eta d\xi \\ &= \int_0^1 \left[r_1\eta + (r_2 - r_1)\xi\eta + \frac{1}{2}(r_3 - r_1)\eta^2 \right]_{\eta=0}^{\eta=1-\xi} d\xi \\ &= \int_0^1 \left[r_1(1-\xi) + (r_2 - r_1)\xi(1-\xi) + \frac{1}{2}(r_3 - r_1)(1-\xi)^2 \right] d\xi \\ &= \int_0^1 \left[(\frac{r_1}{2} + \frac{r_3}{2}) + \xi(r_2 - r_1 - r_3) + \xi^2(-r_2 + \frac{r_1}{2} + \frac{r_3}{2}) \right] d\xi \\ &= \left[(\frac{r_1}{2} + \frac{r_3}{2})\xi + \frac{\xi^2}{2}(r_2 - r_1 - r_3) + \frac{\xi^3}{3}(-r_2 + \frac{r_1}{2} + \frac{r_3}{2}) \right]_{\xi=0}^{\xi=1} \\ &= \frac{3r_1 + 3r_3 + 3r_2 - 3r_1 - 3r_3 - 2r_2 + r_1 + r_3}{6} \\ &= \frac{r_1 + r_2 + r_3}{6} \end{aligned}$$

such that

$$a_i = \frac{r_1 + r_2 + r_3}{12|\Omega_j|} \begin{bmatrix} z_2 - z_3 & r_3 - r_2 \\ z_3 - z_1 & r_1 - r_3 \\ z_1 - z_2 & r_2 - r_1 \end{bmatrix} \begin{bmatrix} z_2 - z_3 & z_3 - z_1 & z_1 - z_2 \\ r_3 - r_2 & r_1 - r_3 & r_2 - r_1 \end{bmatrix}$$

with $2|\Omega_j| = (r_2 - r_1)(z_3 - z_1) - (r_3 - r_1)(z_2 - z_1)$.

In conclusion, the parameters K_u and K_v in the system of equations (2) are given by

$$K_u = \frac{r_1 + r_2 + r_3}{12|\Omega_j|} \begin{bmatrix} z_2 - z_3 & r_3 - r_2 \\ z_3 - z_1 & r_1 - r_3 \\ z_1 - z_2 & r_2 - r_1 \end{bmatrix} \begin{bmatrix} \sigma_{u,r}(z_2 - z_3) & \sigma_{u,r}(z_3 - z_1) & \sigma_{u,r}(z_1 - z_2) \\ \sigma_{u,z}(r_3 - r_2) & \sigma_{u,z}(r_1 - r_3) & \sigma_{u,z}(r_2 - r_1) \end{bmatrix}$$
$$K_v = \frac{r_1 + r_2 + r_3}{12|\Omega_j|} \begin{bmatrix} z_2 - z_3 & r_3 - r_2 \\ z_3 - z_1 & r_1 - r_3 \\ z_1 - z_2 & r_2 - r_1 \end{bmatrix} \begin{bmatrix} \sigma_{v,r}(z_2 - z_3) & \sigma_{v,r}(z_3 - z_1) & \sigma_{v,r}(z_1 - z_2) \\ \sigma_{v,z}(r_3 - r_2) & \sigma_{v,z}(r_1 - r_3) & \sigma_{v,z}(r_2 - r_1) \end{bmatrix}$$

with $(r_1, z_1), (r_2, z_2), (r_3, z_3)$ the vertices of the triangle Ω_j related to c_i.

1.3 Second part of system (2)

For the second part of our system, we have

$$\begin{cases} f_u = -\int_\Omega r R_u(C_u, C_v)\varphi(r, z) d\Omega \\ f_v = \int_\Omega r R_v(C_u, C_v)\varphi(r, z) d\Omega \end{cases}$$

where the definition of the respiration kinetics are known as

$$\begin{cases} R_u(C_u, C_v) = \dfrac{V_{mu} C_u}{(K_{mu} + C_u)(1 + \frac{C_v}{K_{mv}})} \\ R_v(C_u, C_v) = r_q R_u(C_u, C_v) + \dfrac{V_{mfv}}{1 + \frac{C_u}{K_{mfu}}} \end{cases}$$

To allow the simplification of the integrals, we can proceed to the abstraction of some parts of the expressions for R_u and R_v. We make the assumptions that $C_u \ll K_{mfu}$, $C_u \ll K_{mu}$ and $C_v \ll K_{mv}$, simplifying the expressions to

$$\begin{cases} R_u(C_u, C_v) \approx \dfrac{V_{mu} C_u}{K_{mu}} \\ R_v(C_u, C_v) \approx r_q R_u(C_u, C_v) + V_{mfv} \end{cases}$$

which makes them linear functions of the concentrations C_u and C_v.

Going back to the integrals, we have

$$\begin{cases} f_u = -\dfrac{V_{mu}}{K_{mu}} \displaystyle\int_\Omega r C_u \varphi(r,z) d\Omega \\ f_v = -r_q f_u + V_{mfv} \displaystyle\int_\Omega r\varphi(r,z) d\Omega \end{cases}$$

where

$$\begin{aligned} f_u &= -\frac{V_{mu}}{K_{mu}} \int_\Omega r C_u \varphi(r,z) d\Omega \\ &\approx -\frac{V_{mu}}{K_{mu}} \sum_{i=1}^{M} c_i \int_\Omega r(\varphi_i(r,z) \cdot \varphi(r,z)) d\Omega \\ &= -\frac{V_{mu}}{K_{mu}} \sum_{i=1}^{M} c_i \int_0^1 \int_0^{1-\xi} (r_1 + (r_2 - r_1)\xi + (r_3 - r_1)\eta) \begin{bmatrix} 1-\xi-\eta \\ \xi \\ \eta \end{bmatrix} \begin{bmatrix} 1-\xi-\eta \\ \xi \\ \eta \end{bmatrix}^T 2|\Omega_j| d\eta d\xi \end{aligned}$$

Where $(r_1, z_1), (r_2, z_2), (r_3, z_3)$ are the vertices of the triangle Ω_j related to c_i and the area $2|\Omega_j| = (r_2 - r_1)(z_3 - z_1) - (r_3 - r_1)(z_2 - z_1)$. Now we analyse (with $a = 1 - \xi$, $b = r_1 + (r_2 - r_1)\xi$ and $c = r_3 - r_1$)

$$\begin{aligned} &\int_0^{1-\xi} (r_1 + (r_2 - r_1)\xi + (r_3 - r_1)\eta) \begin{bmatrix} (1-\xi-\eta)^2 & (1-\xi-\eta)\xi & (1-\xi-\eta)\eta \\ (1-\xi-\eta)\xi & \xi^2 & \xi\eta \\ (1-\xi-\eta)\eta & \eta\xi & \eta^2 \end{bmatrix} d\eta \\ &= \int_0^{1-\xi} (b + c\eta) \begin{bmatrix} (a-\eta)^2 & (a-\eta)\xi & (a-\eta)\eta \\ (a-\eta)\xi & \xi^2 & \xi\eta \\ (a-\eta)\eta & \eta\xi & \eta^2 \end{bmatrix} d\eta \\ &= \int_0^{1-\xi} \begin{bmatrix} a^2 b + \eta(a^2 c - 2ab) + \eta^2(b - 2ac) + \eta^3 c & (ab + \eta(ac - b) - c\eta^2)\xi & ab\eta + \eta^2(ac - b) - c\eta^3 \\ & (b + c\eta)\xi^2 & (b\eta + c\eta^2)\xi \\ \mathit{Symmetric} & & b\eta^2 + c\eta^3 \end{bmatrix} d\eta \\ &= \begin{bmatrix} a^2 b\eta + \frac{\eta^2}{2}(a^2 c - 2ab) + \frac{\eta^3}{3}(b - 2ac) + \frac{\eta^4}{4}c & (ab\eta + \frac{\eta^2}{2}(ac - b) - \frac{\eta^3}{3}c)\xi & ab\frac{\eta^2}{2} + \frac{\eta^3}{3}(ac - b) - \frac{\eta^4}{4}c \\ & (b\eta + c\frac{\eta^2}{2})\xi^2 & (b\frac{\eta^2}{2} + c\frac{\eta^3}{3})\xi \\ \mathit{Symmetric} & & b\frac{\eta^3}{3} + c\frac{\eta^4}{4} \end{bmatrix}_{\eta=0}^{\eta=a} \\ &= \begin{bmatrix} \frac{1}{12}a^4 c + \frac{1}{3}a^3 b & (\frac{1}{6}a^3 c + \frac{1}{2}a^2 b)\xi & \frac{1}{6}a^3 b + \frac{1}{12}a^4 c) \\ & (ab + c\frac{a^2}{2})\xi^2 & (b\frac{a^2}{2} + c\frac{a^3}{3})\xi \\ \mathit{Symmetric} & & b\frac{a^3}{3} + c\frac{a^4}{4} \end{bmatrix} \end{aligned}$$

We integrate all terms on their own on da with a going from 0 to 1.

$$\begin{aligned} \int_0^1 (\frac{1}{12}a^4 c + \frac{1}{3}a^3 b) d\xi &= \int_0^1 (\frac{1}{12}a^4 c - \frac{1}{3}a^4 r_2 + \frac{1}{3}a^4 r_1 + \frac{1}{3}a^3 r_2) da \\ &= \left[\tfrac{1}{60}a^5 c - \tfrac{1}{15}a^5 r_2 + \tfrac{1}{15}a^5 r_1 + \tfrac{1}{12}a^4 r_2\right]_{a=0}^{a=1} \\ &= \frac{1}{60}(r_3 - r_1) - \frac{1}{15}r_2 + \frac{1}{15}r_1 + \frac{1}{12}r_2 \\ &= \frac{3r_1 + r_2 + r_3}{60} \end{aligned}$$

$$
\begin{aligned}
\int_0^1 ((\frac{1}{6}a^3c+\frac{1}{2}a^2b)\xi)d\xi &= \int_0^1 (\frac{1}{6}a^3c+\frac{1}{2}a^3r_1-\frac{1}{2}a^3r_2+\frac{1}{2}a^4r_2-\frac{1}{6}a^4c-\frac{1}{2}a^4r_1-\frac{1}{2}a^3r_2+\frac{1}{2}a^2r_2)da \\
&= \left[\tfrac{1}{24}a^4c+\tfrac{1}{8}a^4r_1-\tfrac{1}{8}a^4r_2+\tfrac{1}{10}a^5r_2-\tfrac{1}{30}a^5c-\tfrac{1}{10}a^5r_1-\tfrac{1}{8}a^4r_2+\tfrac{1}{6}a^3r_2\right]_{a=0}^{a=1} \\
&= \frac{1}{24}c+\frac{1}{8}r_1-\frac{1}{8}r_2+\frac{1}{10}r_2-\frac{1}{30}c-\frac{1}{10}r_1-\frac{1}{8}r_2+\frac{1}{6}r_2 \\
&= \frac{2r_1+2r_2+r_3}{120}
\end{aligned}
$$

$$
\begin{aligned}
\int_0^1 (\frac{1}{6}a^3b+\frac{1}{12}a^4c)d\xi &= \int_0^1 (\frac{1}{12}a^4c+\frac{1}{6}r_1a^4+\frac{1}{6}r_2a^3-\frac{1}{6}r_2a^4)da \\
&= \left[\tfrac{1}{60}a^5c+\tfrac{1}{30}r_1a^5+\tfrac{1}{24}r_2a^4-\tfrac{1}{30}r_2a^5\right]_{a=0}^{a=1} \\
&= \frac{1}{60}c+\frac{1}{30}r_1+\frac{1}{24}r_2-\frac{1}{30}r_2 \\
&= \frac{2r_1+r_2+2r_3}{120}
\end{aligned}
$$

$$
\int_0^1 ((ab+c\frac{a^2}{2})\xi^2)d\xi = \frac{r_1+3r_2+r_3}{60}
$$

$$
\int_0^1 ((b\frac{a^2}{2}+c\frac{a^3}{3})\xi)d\xi = \frac{r_1+2r_2+2r_3}{120}
$$

$$
\begin{aligned}
\int_0^1 (b\frac{a^3}{3}+c\frac{a^4}{4})d\xi &= \int_0^1 (\frac{1}{3}r_1a^4+\frac{1}{3}r_2a^3-\frac{1}{3}r_2a^4+\frac{1}{4}ca^4)da \\
&= \frac{r_1+r_2+3r_3}{60}
\end{aligned}
$$

which brings us to

$$
\begin{aligned}
f_u &= -\frac{2|\Omega_j|V_{mu}}{K_{mu}}\sum_{i=1}^{M} c_i \frac{1}{120}\begin{bmatrix} 6r_1+2r_2+2r_3 & 2r_1+2r_2+r_3 & 2r_1+r_2+2r_3 \\ 2r_1+2r_2+r_3 & 2r_1+6r_2+2r_3 & r_1+2r_2+2r_3 \\ 2r_1+r_2+2r_3 & r_1+2r_2+2r_3 & 2r_1+2r_2+6r_3 \end{bmatrix} \\
&= -\frac{|\Omega_j|V_{mu}}{60K_{mu}}\sum_{i=1}^{M} c_i \begin{bmatrix} 6r_1+2r_2+2r_3 & 2r_1+2r_2+r_3 & 2r_1+r_2+2r_3 \\ 2r_1+2r_2+r_3 & 2r_1+6r_2+2r_3 & r_1+2r_2+2r_3 \\ 2r_1+r_2+2r_3 & r_1+2r_2+2r_3 & 2r_1+2r_2+6r_3 \end{bmatrix}
\end{aligned}
$$

and for f_v we still need to calculate

$$
\begin{aligned}
\int_\Omega r\varphi(r,z)d\Omega &= \int_0^1 \int_0^{1-\xi} (r_1 + (r_2 - r_1)\xi + (r_3 - r_1)\eta) \begin{bmatrix} 1-\xi-\eta \\ \xi \\ \eta \end{bmatrix} 2|\Omega_j| d\eta d\xi \\
&= 2|\Omega_j| \int_0^1 \int_0^a \begin{bmatrix} (b+c\eta)(a-\eta) \\ (b+c\eta)\xi \\ (b+c\eta)\eta \end{bmatrix} d\eta d\xi \\
&= 2|\Omega_j| \int_0^1 \begin{bmatrix} ab\eta + \frac{1}{2}\eta^2(ac-b) - \frac{1}{3}c\eta^3 \\ b\xi\eta + \frac{1}{2}c\eta^2\xi \\ \frac{1}{2}b\eta^2 + \frac{1}{3}c\eta^3 \end{bmatrix}_{\eta=0}^{\eta=a} d\xi \\
&= 2|\Omega_j| \int_0^1 \begin{bmatrix} a^2b + \frac{1}{2}a^2(ac-b) - \frac{1}{3}ca^3 \\ b(1-a)a + \frac{1}{2}ca^2(1-a) \\ \frac{1}{2}ba^2 + \frac{1}{3}ca^3 \end{bmatrix} da \\
&= 2|\Omega_j| \int_0^1 \begin{bmatrix} \frac{1}{6}a^3c \\ ab - a^2b + \frac{1}{2}(ca^2 - ca^3) \\ \frac{1}{2}ba^2 + \frac{1}{3}ca^3 \end{bmatrix} da \\
&= 2|\Omega_j| \int_0^1 \begin{bmatrix} \frac{1}{6}a^3c \\ r_1a^2 + r_2a - 2r_2a^2 - r_1a^3 + r_2a^3 + \frac{1}{2}(ca^2 - ca^3) \\ \frac{1}{2}(r_1a^3 + r_2a^2 - r_2a^3) + \frac{1}{3}ca^3 \end{bmatrix} da \\
&= 2|\Omega_j| \begin{bmatrix} \frac{1}{24}a^4c \\ \frac{1}{3}r_1a^3 + \frac{1}{2}r_2a^2 - \frac{1}{3}2r_2a^3 - \frac{1}{4}r_1a^4 + \frac{1}{4}r_2a^4 + \frac{1}{6}ca^3 - \frac{1}{8}ca^4) \\ \frac{1}{8}r_1a^4 + \frac{1}{6}r_2a^3 - \frac{1}{8}r_2a^4 + \frac{1}{12}ca^4 \end{bmatrix}_{a=0}^{a=1} \\
&= \frac{1}{12}|\Omega_j| \begin{bmatrix} r_3 - r_1 \\ r_1 + 2r_2 + r_3 \\ r_1 + r_2 + 2r_3 \end{bmatrix}
\end{aligned}
$$

1.4 Third part of system (2)

Concerning the boundary conditions of our system, we have the following:

$$\begin{cases} H_u(c_u, c_v) = \int_\Gamma r\rho_u C_u^*(r,z)\varphi(r,z)d\Gamma \\ H_v(c_u, c_v) = \int_\Gamma r\rho_v C_v^*(r,z)\varphi(r,z)d\Gamma \end{cases}$$

Now, since the functions C^* are zero on Γ_1, and that these equations are symmetrical w.r.t. u and v, we only consider the following equation:

$$\begin{aligned} H_u(c_u, c_v) &= \int_{\Gamma_2} r\rho_u(C_u(r,z) - C_{u\text{amb}})\varphi(r,z)d\Gamma \\ &= \int_{\Gamma_2} r\rho_u C_u(r,z)\varphi(r,z)d\Gamma - \int_{\Gamma_2} r\rho_u C_{u\text{amb}}\varphi(r,z)d\Gamma \end{aligned}$$

By making use of the triangulation, we have

$$H_u(c_u, c_v) = \rho_u \sum_{i=1}^{M} c_i \int_{\Gamma_j} r(\varphi_i(r,z)\cdot\varphi(r,z))d\Gamma - \rho_u C_{u\text{amb}} \int_{\Gamma_j} r\varphi(r,z)d\Gamma$$

with Γ_j the part of Γ_2 related to c_i. Since we are working on the boundary, we must only work with edges between two vertices and thus the new basis functions can be given by

$$\begin{aligned} \psi_1(\xi,\eta) &= 1 - \xi \\ \psi_2(\xi,\eta) &= \xi \end{aligned}$$

with

$$\begin{aligned} r &= r_1 + (r_2 - r_1)\xi \\ z &= z_1 + (z_2 - z_1)\xi \end{aligned}$$

This gives us

$$\begin{aligned} \int_{\Gamma_j} r(\varphi_i(r,z)\cdot\varphi(r,z))d\Gamma &= |\Gamma_j| \int_0^1 (r_1 + (r_2 - r_1)\xi) \begin{bmatrix} 1-\xi \\ \xi \end{bmatrix} \begin{bmatrix} 1-\xi & \xi \end{bmatrix} d\xi \\ &= |\Gamma_j| \int_0^1 (r_1 + (r_2 - r_1)\xi) \begin{bmatrix} 1 - 2\xi + \xi^2 & \xi - \xi^2 \\ \xi - \xi^2 & \xi^2 \end{bmatrix} d\xi \end{aligned}$$

$$\begin{aligned} &= |\Gamma_j| \begin{bmatrix} \frac{1}{4}(r_2 - r_1) + \frac{1}{3}(3r_1 - 2r_2) + \frac{1}{2}(-3r_1 + r_2) + r_1 & \frac{1}{4}(r_1 - r_2) - \frac{1}{3}r_1 + \frac{1}{3}(r_2 - r_1) + \frac{1}{2}r_1 \\ \frac{1}{4}(r_1 - r_2) - \frac{1}{3}r_1 + \frac{1}{3}(r_2 - r_1) + \frac{1}{2}r_1 & \frac{1}{4}(r_2 - r_1) + \frac{1}{3}r_1 \end{bmatrix} \\ &= |\Gamma_j| \begin{bmatrix} \frac{r_1}{4} + \frac{r_2}{12} & \frac{r_1}{12} + \frac{r_2}{12} \\ \frac{r_1}{12} + \frac{r_2}{12} & \frac{r_1}{12} + \frac{r_2}{4} \end{bmatrix} \\ &= \frac{|\Gamma_j|}{12} \begin{bmatrix} 3r_1 + r_2 & r_1 + r_2 \\ r_1 + r_2 & r_1 + 3r_2 \end{bmatrix} \end{aligned}$$

The other integral is given by

$$\begin{aligned}
\int_{\Gamma_j} r\varphi(r,z)d\Gamma &= |\Gamma_j| \int_0^1 (r_1 + (r_2 - r_1)\xi) \begin{bmatrix} 1-\xi \\ \xi \end{bmatrix} d\xi \\
&= |\Gamma_j| \int_0^1 \begin{bmatrix} r_1 + (r_2 - 2r_1)\xi + (r_1 - r_2)\xi^2 \\ r_1\xi + (r_2 - r_1)\xi^2 \end{bmatrix} d\xi \\
&= |\Gamma_j| \begin{bmatrix} r_1\xi + \frac{1}{2}(r_2 - 2r_1)\xi^2 + \frac{1}{3}(r_1 - r_2)\xi^3 \\ \frac{1}{2}r_1\xi^2 + \frac{1}{3}(r_2 - r_1)\xi^3 \end{bmatrix}_{\xi=0}^{\xi=1} \\
&= |\Gamma_j| \begin{bmatrix} \frac{r_1}{3} + \frac{r_2}{6} \\ \frac{r_1}{6} + \frac{r_2}{3} \end{bmatrix} \\
&= \frac{|\Gamma_j|}{6} \begin{bmatrix} 2r_1 + r_2 \\ r_1 + 2r_2 \end{bmatrix}
\end{aligned}$$

We thus get the following final equations:

$$\begin{aligned}
H_u(c_u, c_v) &= \rho_u \sum_{i=1}^{M} c_i \Big(\frac{|\Gamma_j|}{12} \begin{bmatrix} 3r_1 + r_2 & r_1 + r_2 \\ r_1 + r_2 & r_1 + 3r_2 \end{bmatrix} \Big) - \rho_u C_{u\text{amb}} \Big(\frac{|\Gamma_j|}{6} \begin{bmatrix} 2r_1 + r_2 \\ r_1 + 2r_2 \end{bmatrix} \Big) \\
H_v(c_u, c_v) &= \rho_v \sum_{i=1}^{M} c_{M+i} \Big(\frac{|\Gamma_j|}{12} \begin{bmatrix} 3r_1 + r_2 & r_1 + r_2 \\ r_1 + r_2 & r_1 + 3r_2 \end{bmatrix} \Big) - \rho_v C_{v\text{amb}} \Big(\frac{|\Gamma_j|}{6} \begin{bmatrix} 2r_1 + r_2 \\ r_1 + 2r_2 \end{bmatrix} \Big)
\end{aligned}$$

with

$$|\Gamma_j| = \sqrt{(r_1 - r_2)^2 + (z_1 - z_2)^2}$$

the length of the boundary between (r_1, z_1) and (r_2, z_2).

In conclusion, the system that we need to solve is the following

$$\begin{pmatrix} K_u & 0 \\ 0 & K_v \end{pmatrix} \begin{pmatrix} c_u \\ c_v \end{pmatrix} - \begin{pmatrix} f_u \\ f_v \end{pmatrix} + \begin{pmatrix} H_u(c_u, c_v) \\ H_v(c_u, c_v) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

where the different parameters in Ω are given by

$$K_u = \frac{r_1 + r_2 + r_3}{12|\Omega_j|} \begin{bmatrix} z_2 - z_3 & r_3 - r_2 \\ z_3 - z_1 & r_1 - r_3 \\ z_1 - z_2 & r_2 - r_1 \end{bmatrix} \begin{bmatrix} \sigma_{u,r}(z_2 - z_3) & \sigma_{u,r}(z_3 - z_1) & \sigma_{u,r}(z_1 - z_2) \\ \sigma_{u,z}(r_3 - r_2) & \sigma_{u,z}(r_1 - r_3) & \sigma_{u,z}(r_2 - r_1) \end{bmatrix}$$

$$K_v = \frac{r_1 + r_2 + r_3}{12|\Omega_j|} \begin{bmatrix} z_2 - z_3 & r_3 - r_2 \\ z_3 - z_1 & r_1 - r_3 \\ z_1 - z_2 & r_2 - r_1 \end{bmatrix} \begin{bmatrix} \sigma_{v,r}(z_2 - z_3) & \sigma_{v,r}(z_3 - z_1) & \sigma_{v,r}(z_1 - z_2) \\ \sigma_{v,z}(r_3 - r_2) & \sigma_{v,z}(r_1 - r_3) & \sigma_{v,z}(r_2 - r_1) \end{bmatrix}$$

$$f_u = -\frac{|\Omega_j| V_{mu}}{60 K_{mu}} \sum_{i=1}^{M} c_i \begin{bmatrix} 6r_1 + 2r_2 + 2r_3 & 2r_1 + 2r_2 + r_3 & 2r_1 + r_2 + 2r_3 \\ 2r_1 + 2r_2 + r_3 & 2r_1 + 6r_2 + 2r_3 & r_1 + 2r_2 + 2r_3 \\ 2r_1 + r_2 + 2r_3 & r_1 + 2r_2 + 2r_3 & 2r_1 + 2r_2 + 6r_3 \end{bmatrix}$$

$$f_v = \frac{r_q |\Omega_j| V_{mu}}{60 K_{mu}} \sum_{i=1}^{M} c_i \begin{bmatrix} 6r_1 + 2r_2 + 2r_3 & 2r_1 + 2r_2 + r_3 & 2r_1 + r_2 + 2r_3 \\ 2r_1 + 2r_2 + r_3 & 2r_1 + 6r_2 + 2r_3 & r_1 + 2r_2 + 2r_3 \\ 2r_1 + r_2 + 2r_3 & r_1 + 2r_2 + 2r_3 & 2r_1 + 2r_2 + 6r_3 \end{bmatrix} + \frac{V_{mfv}}{12} |\Omega_j| \begin{bmatrix} r_3 - r_1 \\ r_1 + 2r_2 + r_3 \\ r_1 + r_2 + 2r_3 \end{bmatrix}$$

with $(r_1, z_1), (r_2, z_2), (r_3, z_3)$ the vertices of the triangle Ω_j related to c_i and with $2|\Omega_j| = (r_2 - r_1)(z_3 - z_1) - (r_3 - r_1)(z_2 - z_1)$.

On the boundary Γ_2, we have

$$H_u(c_u, c_v) = \rho_u \sum_{i=1}^{M} c_i \Big(\frac{|\Gamma_j|}{12} \begin{bmatrix} 3r_1 + r_2 & r_1 + r_2 \\ r_1 + r_2 & r_1 + 3r_2 \end{bmatrix} \Big) - \rho_u C_{u\mathrm{amb}} \Big(\frac{|\Gamma_j|}{6} \begin{bmatrix} 2r_1 + r_2 \\ r_1 + 2r_2 \end{bmatrix} \Big)$$

$$H_v(c_u, c_v) = \rho_v \sum_{i=1}^{M} c_{M+i} \Big(\frac{|\Gamma_j|}{12} \begin{bmatrix} 3r_1 + r_2 & r_1 + r_2 \\ r_1 + r_2 & r_1 + 3r_2 \end{bmatrix} \Big) - \rho_v C_{v\mathrm{amb}} \Big(\frac{|\Gamma_j|}{6} \begin{bmatrix} 2r_1 + r_2 \\ r_1 + 2r_2 \end{bmatrix} \Big)$$

with

$$|\Gamma_j| = \sqrt{(r_1 - r_2)^2 + (z_1 - z_2)^2}$$

the length of the boundary between (r_1, z_1) and (r_2, z_2).

On the boundary Γ_1, we have

$$H_u(c_u, c_v) = 0$$
$$H_v(c_u, c_v) = 0$$

Corresponding names in C++ code

$$K_u = \frac{r_1+r_2+r_3}{12|\Omega_j|}\begin{bmatrix} z_2-z_3 & r_3-r_2 \\ z_3-z_1 & r_1-r_3 \\ z_1-z_2 & r_2-r_1 \end{bmatrix}\begin{bmatrix} \sigma_{u,r}(z_2-z_3) & \sigma_{u,r}(z_3-z_1) & \sigma_{u,r}(z_1-z_2) \\ \sigma_{u,z}(r_3-r_2) & \sigma_{u,z}(r_1-r_3) & \sigma_{u,z}(r_2-r_1) \end{bmatrix}$$

$$K_v = \frac{r_1+r_2+r_3}{12|\Omega_j|}\begin{bmatrix} z_2-z_3 & r_3-r_2 \\ z_3-z_1 & r_1-r_3 \\ z_1-z_2 & r_2-r_1 \end{bmatrix}\begin{bmatrix} \sigma_{v,r}(z_2-z_3) & \sigma_{v,r}(z_3-z_1) & \sigma_{v,r}(z_1-z_2) \\ \sigma_{v,z}(r_3-r_2) & \sigma_{v,z}(r_1-r_3) & \sigma_{v,z}(r_2-r_1) \end{bmatrix}$$

$$f_u = -\frac{|\Omega_j|}{60}\begin{bmatrix} 6r_1+2r_2+2r_3 & 2r_1+2r_2+r_3 & 2r_1+r_2+2r_3 \\ 2r_1+2r_2+r_3 & 2r_1+6r_2+2r_3 & r_1+2r_2+2r_3 \\ 2r_1+r_2+2r_3 & r_1+2r_2+2r_3 & 2r_1+2r_2+6r_3 \end{bmatrix}$$

$$f_{v1} = \frac{|\Omega_j|}{60}\begin{bmatrix} 6r_1+2r_2+2r_3 & 2r_1+2r_2+r_3 & 2r_1+r_2+2r_3 \\ 2r_1+2r_2+r_3 & 2r_1+6r_2+2r_3 & r_1+2r_2+2r_3 \\ 2r_1+r_2+2r_3 & r_1+2r_2+2r_3 & 2r_1+2r_2+6r_3 \end{bmatrix}$$

$$f_{v2} = \frac{|\Omega_j|}{12}\begin{bmatrix} r_3-r_1 \\ r_1+2r_2+r_3 \\ r_1+r_2+2r_3 \end{bmatrix}$$

$$H_{u1} = \rho_u\Big(\frac{|\Gamma_j|}{12}\begin{bmatrix} 3r_1+r_2 & r_1+r_2 \\ r_1+r_2 & r_1+3r_2 \end{bmatrix}\Big)$$

$$H_{u2} = \rho_u C_{u\text{amb}}\Big(\frac{|\Gamma_j|}{6}\begin{bmatrix} 2r_1+r_2 \\ r_1+2r_2 \end{bmatrix}\Big)$$

$$H_{v1} = \rho_v\Big(\frac{|\Gamma_j|}{12}\begin{bmatrix} 3r_1+r_2 & r_1+r_2 \\ r_1+r_2 & r_1+3r_2 \end{bmatrix}\Big)$$

$$H_{v2} = \rho_v C_{v\text{amb}}\Big(\frac{|\Gamma_j|}{6}\begin{bmatrix} 2r_1+r_2 \\ r_1+2r_2 \end{bmatrix}\Big)$$

The linear equations are thus given by

$$K_u c_u - \frac{V_{mu}}{K_{mu}} f_u c_u + H_{u1} c_u - H_{u2}$$
$$K_v c_v - r_q f_{v1} c_u - V_{mfv} f_{v2} + H_{v1} c_v - H_{v2}$$

Bringing back the non-linearity introduced by the functions R_u and R_v, we get

$$K_u c_u - f_u R_u(c_u, c_v) + H_{u1} c_u - H_{u2}$$
$$K_v c_v - f_{v1} R_v(c_u, c_v) + H_{v1} c_v - H_{v2}$$

with

$$\begin{cases} R_u(C_u, C_v) = \dfrac{V_{mu} C_u}{(K_{mu}+C_u)(1+\frac{C_v}{K_{mv}})} \\ R_v(C_u, C_v) = r_q R_u(C_u, C_v) + \dfrac{V_{mfv}}{1+\frac{C_u}{K_{mfu}}} \end{cases}$$

which means that the function f_{v2} is not used anymore, it is only necessary for the linear case to find the initial values.