Exercise 1 to section 4.2

Derive and plot vectors describing reaction stoichiometry and kinetics for the reacting mixture NO_2 and N_2O_4. Consider orthonormal bases $\vec{e}^{\alpha} = \vec{e}_{\alpha}$.

Try to answer before continuing reading.

Numbering of the two components ($n = 2$, the space $\mathcal{U}$ is thus 2-dimensional): $1 = NO_2$, $2 = N_2O_4$. The (composition) matrix $\|T_{\sigma\alpha}\|$ is

$$\begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}$$

and its rank (h) is one; the number of independent reactions is thus $n - h = 1$. The matrix $\|S_{\sigma\alpha}\|$ can be then selected as

$$\begin{pmatrix} 1 & 2 \end{pmatrix}.$$

The "atomic" substance E^{σ} is thus NO_2.

The vector of molar masses is

$$\vec{M} = M_{\mathrm{NO_2}}\vec{e}^{1} + \vec{M}_{\mathrm{N_2O_4}}\vec{e}^{2}.$$

The basis vector of the 1-dimensional subspace $\mathcal{W}$ is

$$\vec{f}_1 = \vec{e}^{1} + 2\vec{e}^{2}.$$

The stoichiometric matrix of the only one independent reaction can be selected as

$$\|P_{p\alpha}\| = \begin{pmatrix} -2 & 1 \end{pmatrix}$$

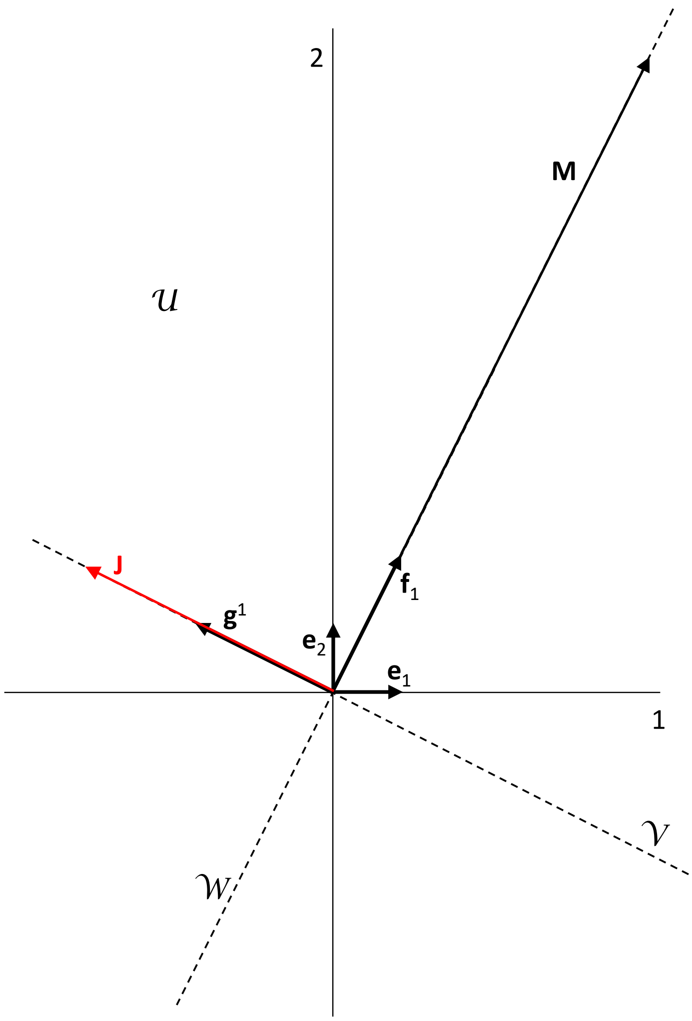
and the corresponding independent reaction is $2NO_2 = N_2O_4$. Thus the basis vector of the 1-dimensional reaction subspace $\mathcal{V}$ is

$$\vec{g}^{1} = -2\vec{e}_1 + \vec{e}_2.$$

The vector of reaction rates can be written in terms of the independent rate or component rates:

$$\vec{J} = J_1\vec{g}^{1} = J^1\vec{e}_1 + J^2\vec{e}_2.$$

The spaces and vectors are shown in the figure below. The vector of molar masses is drawn in units of dag/mol to fit the available space; for example NO_2 has the molar weight of 4.6 dag/mol. An example of the reaction rate vector is drawn in red for the case of $J^1 = -4$, then $J^2 = 2$ as follows from (4.20) and (4.26), and $J_1 = 2$ as follows from (4.45). The relationship between the reaction rate and the component rates, which is given by eq. (4.45) in the book, contains the covariant metric sensor g_{rp}. The latter tensor is obtained by the inversion of the contravariant metric tensor $g^{rp} = \vec{g}^{r}.\vec{g}^{p}$. In our case $g^{11} = \vec{g}^{1}.\vec{g}^{1} = 5$ and $g_{11} = 1/5$. Then $J_1 = J^1(-2)(1/5) + J^2(1/5)$.


2
M
𝒰
J
$\mathbf{f}_1$
$\mathbf{g}^1$
$\mathbf{e}_2$
$\mathbf{e}_1$
1
𝒱
𝒲