

The Jacobian element $J_{i,s}$ is still:

$$J_{i,s} = \frac{\partial \dot{n}_i}{\partial n_s}$$

but now $\dot{n}_i = V \sum_j \nu_{ij} \cdot k_j \prod_r C_r^{(j)}$ where $V = V(n_{tot})$ is no longer constant, and $C_r = n_r/V(n_{tot})$ also depends on all mole numbers through V . So the derivative is more involved:

$$J_{i,s} = \sum_j \nu_{ij} \cdot k_j \cdot \frac{\partial}{\partial n_s} \left(V \prod_r C_r^{(j)} \right)$$

Since $C_r = n_r/V$ and $V = nRT/P$, the product $V \prod_r C_r^{(j)}$ for a bimolecular reaction $A + B$ is:

$$V \cdot C_A \cdot C_B = V \cdot \frac{n_A}{V} \cdot \frac{n_B}{V} = \frac{n_A n_B}{V} = \frac{n_A n_B P}{n_{tot} RT}$$

So differentiating with respect to n_s :

$$\frac{\partial}{\partial n_s} \left(\frac{n_A n_B}{V} \right) = \frac{\delta_{sA} n_B + \delta_{sB} n_A}{V} - \frac{n_A n_B}{V^2} \frac{\partial V}{\partial n_s}$$

Since $\partial V / \partial n_s = RT/P = V/n_{tot}$ for all s , this gives:

$$= \frac{\delta_{sA} C_B + \delta_{sB} C_A}{1} - \frac{C_A C_B}{C_{tot}}$$

The first term is the **direct** derivative (the `deriv` in the code) and the second term is the **volume correction** (the `corr` in the code), which is the same for every species s and gets broadcast across all columns. The general form for a reaction with any number of reactants is:

$$J_{i,s} = \sum_{j \ni s} \nu_{ij} \cdot k_j \prod_{r \neq s} C_r^{(j)} - \sum_j \nu_{ij} \cdot \frac{k_j}{C_{tot}} \prod_r C_r^{(j)}$$

where:

- The **first sum** runs only over reactions involving s , giving the direct concentration derivative — this is the `deriv` term
- The **second sum** runs over all reactions regardless of whether they involve s , giving the volume-expansion correction — this is the `corr` term, and because it doesn't depend on s it appears in every column of the Jacobian for each affected row i

This is why in the isobaric code the `corr` loops iterate over `for i in range(num_core_species)` — the correction is the same for every column s , so it gets added to the entire row at once.