

# Supporting Information

## Design of Storage Equipment for Unstable Chemicals Using Sensitivity-Based Methods

Giuseppe Andriani<sup>1</sup>, Paolo Mocellin<sup>1,2,\*</sup>, Gianmaria Pio<sup>3</sup>, Ernesto Salzano<sup>3</sup>, Chiara Vianello<sup>1</sup>

<sup>1</sup> Università degli Studi di Padova, Dipartimento di Ingegneria Industriale, Via Marzolo 9, 35131 Padova, Italia.

<sup>2</sup> Università degli Studi di Padova, Dipartimento di Ingegneria Civile, Edile e Ambientale, Via Marzolo 9, 35131 Padova, Italia.

<sup>3</sup> Università di Bologna, Dipartimento di Ingegneria Civile, Chimica, Ambientale e dei Materiali, Via Terracini 28, 40131 Bologna, Italia.

Corresponding author email: [paolo.mocellin@unipd.it](mailto:paolo.mocellin@unipd.it)

In Table S1 are illustrated the dimensionless governing values retrievable with the three different Frank-Kamenetskii theories (Canonical, Expanded and Comprehensive FKT) useful for storage vessels design and verification purposes, for the aqueous solution of 30% w/w hydroxylamine system (HA30). Conversely, Table S2 reports the vessel design parameters as a function of the ambient temperature selected for the HA30 system.

Table S1. HA30 storage system. Critical Frank-Kamenetskii parameter ( $\delta_{crit}$ ) and maximum dimensionless temperature ( $\theta_{max}$ ) as a function of the ambient temperature selected ( $T_{amb}$ ).

| Hydroxylamine<br>30% w/w | Ambient<br>temperature | Dimensionless<br>activation<br>energy | Lewis<br>number | Dimensionless<br>heat of<br>reaction | Critical FK<br>parameter | Max dimensionless<br>temperature |                             |
|--------------------------|------------------------|---------------------------------------|-----------------|--------------------------------------|--------------------------|----------------------------------|-----------------------------|
|                          | $T_{amb}$ [K]          | $\gamma$ [-]                          | $Le$<br>[-]     | $B$ [-]                              | $\delta_{crit}$ [-]      | $\theta_{max} \delta_{crit}$ [-] | $\theta_{max} \delta=2$ [-] |
| Canonical FKT            | 278.15                 | -                                     | -               | -                                    |                          |                                  |                             |
|                          | 293.15                 | -                                     | -               | -                                    | 2.00                     | 1.39                             | 1.39                        |
|                          | 308.15                 | -                                     | -               | -                                    |                          |                                  |                             |
| Extended FKT             | 278.15                 | 45.46                                 | -               | -                                    | 2.05                     | 1.46                             | 1.15                        |
|                          | 293.15                 | 43.13                                 | -               | -                                    | 2.05                     | 1.48                             | 1.14                        |
|                          | 308.15                 | 41.03                                 | -               | -                                    | 2.06                     | 1.48                             | 1.14                        |
| Comprehensive<br>FKT     | 278.15                 | 45.46                                 | 56.45           | 30.80                                | 2.71                     | 6.98                             | 0.82                        |
|                          | 293.15                 | 43.13                                 | 59.74           | 27.73                                | 2.79                     | 7.30                             | 0.81                        |
|                          | 308.15                 | 41.03                                 | 62.69           | 25.10                                | 2.87                     | 7.42                             | 0.80                        |

Table S2. HA30 storage system. Vessel design parameters as a function of the ambient temperature selected ( $T_{amb}$ ). The onset temperature ( $T_{onset}$ ) of the HA30 system is 405 K.

| Hydroxylamine<br>30% w/w | Ambient<br>temperature | Critical<br>vessel radius | Max temp. at $\delta_{crit}$ | Max temp. at $\delta = 2$ |
|--------------------------|------------------------|---------------------------|------------------------------|---------------------------|
|                          | $T_{amb}$ [K]          | $r_{w,crit}$ [m]          | $T_{max} \delta_{crit}$ [K]  | $T_{max} \delta=2$ [K]    |
| Canonical FKT            | 278.15                 | 6.89                      | 286.63                       | 286.63                    |
|                          | 293.15                 | 2.33                      | 302.57                       | 302.57                    |
|                          | 308.15                 | 0.88                      | 318.56                       | 318.56                    |
| Extended FKT             | 278.15                 | 6.97                      | 287.08                       | 285.15                    |
|                          | 293.15                 | 2.36                      | 303.21                       | 300.89                    |
|                          | 308.15                 | 0.89                      | 319.26                       | 316.67                    |
| Comprehensive<br>FKT     | 278.15                 | 8.02                      | 320.86                       | 283.17                    |
|                          | 293.15                 | 2.76                      | 342.76                       | 298.65                    |
|                          | 308.15                 | 1.05                      | 363.87                       | 314.16                    |

