Absorption column modeling
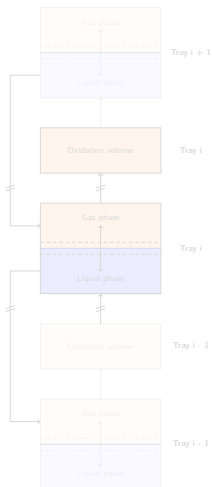
Thermodynamically consistent dynamic model of NO_x absorption column

By: Kjetil Sonerud
Supervisor: Tore Haug-Warberg

October 15, 2014

Project background
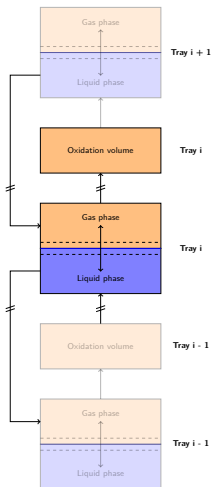## What makes absorption column modeling interesting?

- Industrial relevance: Yara International AS
- Central part of the fertilizer production
  - Production of HNO_3 from NO_x
- Chemically interesting problem
  - Simultaneous absorption, desorption and chemical reaction
  - Complex reaction pathway

"It would be difficult to cite a process so common to industrial chemical scenario and yet posing so severe a challenge to our comprehension of its fundamental mechanism as that of absorption of nitrogen oxides in water to produce nitric acid."

I. B. Chatterjee, J. B. Joshi,
Chemical Engineering Journal 138 (2008) 556-577

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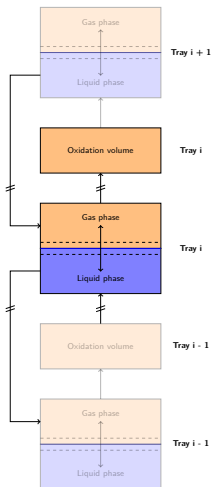What makes absorption column modeling interesting?

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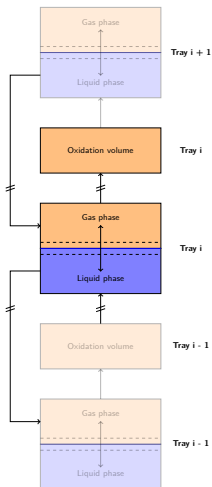
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Project scope
Areas of focus

Key points:

- Thermodynamically consistent mass- and energy balance

- How to avoid an explicit momentum balance in a consistent fashion? (i.e. using a pre-defined pressure profile)

- Integration with Rgrad (thermodynamic framework by THW et al.)

- Expanding from single tray to multiple trays (i.e. realistic example from Yara). How to set this up in a way that promotes robust solvability?

- Set up the model in a way that promotes exploration of the fundamental mechanism of the problem–what are the bottlenecks?

In general: The focus is on the theoretical understanding of the modeling, not the (numeric) implementation itself. If time, MATLAB or Julia will be used to evaluate an example case.

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"Essentially, all models are wrong.
However, some models are rather useful."

George E. P. Box