UNIVERSITY OF TWENTE.

ADVANCED CHEMICAL REACTION ENGINEERING

PART - II

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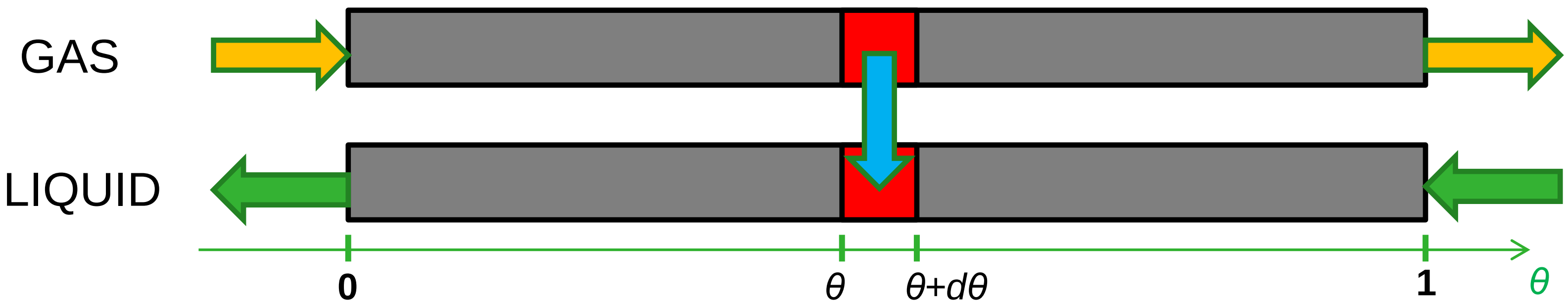
BOUNDARY VALUE PROBLEMS

EXAMPLE: COUNTERCURRENT ABSORPTION



$$\begin{cases} u_g \dfrac{dC_g}{d\theta} + ka\left(C_g - C_l\right) = 0 \\ u_l \dfrac{dC_l}{d\theta} - ka\left(C_g - C_l\right) = 0 \end{cases}$$

$$\begin{cases} \theta = 0 \quad \rightarrow \quad C_g = 1 \\ \theta = 1 \quad \rightarrow \quad C_l = 0 \end{cases}$$

$$y(1) = C_g, \qquad y(2) = C_l$$

N.B. Velocity u_l is negative!

BOUNDARY VALUE PROBLEMS

BVP4C (1)

```
sol = bvp4c (odefun, bcfun, solinit)
```

`odefun` a function that defines the differential equations (similar to ODE45)

`bcfun` a function that defines the “residual” at the boundary conditions.
In other words, the b.c. must be expressed in the form f(y)=0

```
res = bcfun (ya, yb)
```

1st boundary *2nd boundary*

$$\begin{cases} \theta = 0 & \rightarrow \quad y_1 - 1 = 0 \\ \theta = 1 & \rightarrow \quad y_2 = 0 \end{cases} \longrightarrow \quad \text{res} = \begin{bmatrix} \text{ya}(1) - 1 \\ \text{yb}(2) \end{bmatrix}$$

BOUNDARY VALUE PROBLEMS

BVP4C (2)

```
sol = bvp4c (odefun, bcfun, solinit)
```

`solinit` provides the initial conditions

```
solinit = bvpinit (x, yinit)
```

Tentative mesh

Vector of initial values
(one initial value per each variable)

The selected mesh is only an initial guess! The solver will select its own mesh!

BOUNDARY VALUE PROBLEMS
EXERCISE

Exercise. Write a model for the counter-current gas-liquid absorption.

$$\begin{cases} u_g \dfrac{dC_g}{d\theta} + ka\left(C_g - C_l\right) = 0 \\ u_l \dfrac{dC_l}{d\theta} - ka\left(C_g - C_l\right) = 0 \end{cases}$$

$$\begin{cases} \theta = 0 \quad \rightarrow \quad C_g = 1 \\ \theta = 1 \quad \rightarrow \quad C_l = 0 \end{cases}$$