From self-organization to evolution of RNA molecules

The origin of biological information

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Self-formation. Theory and application

Vilnius, 26.– 28.11.2003

Web-Page for further information:

http://www.tbi.univie.ac.at/~pks

1. **Autocatalytic chemical reactions in the flow reactor**

2. **Replication, mutation, selection and Shannon information**

3. **Evolution *in silico* and optimization of RNA structures**

4. **Random walks and ‚ensemble learning‘**

5. **Sequence-structure maps, neutral networks, and intersections**

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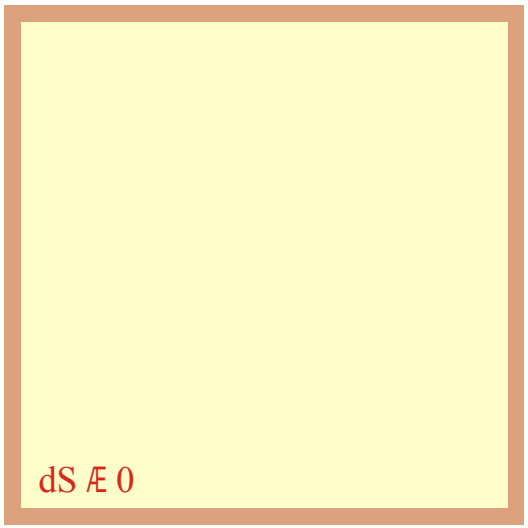
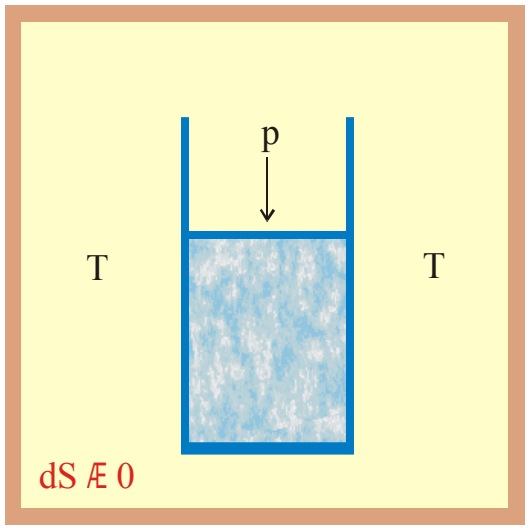
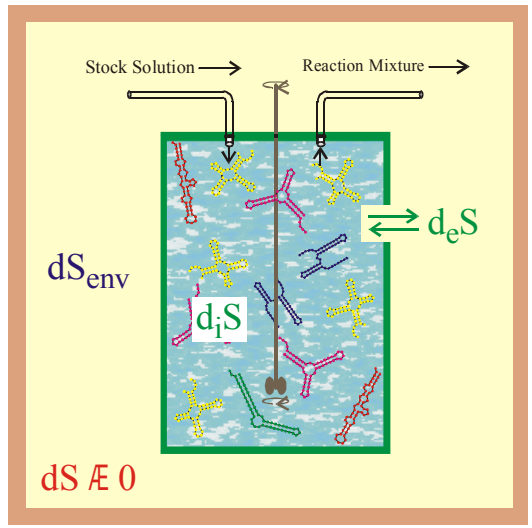






Isolated system

U = const., V = const.,

dS Æ 0

Closed system

T = const., p = const.,

dG = dU-pdV-TdS ¶ 0

Open system

$dS = dS_{env} + dS \text{ Æ } 0$

$dS = d_iS + d_eS$

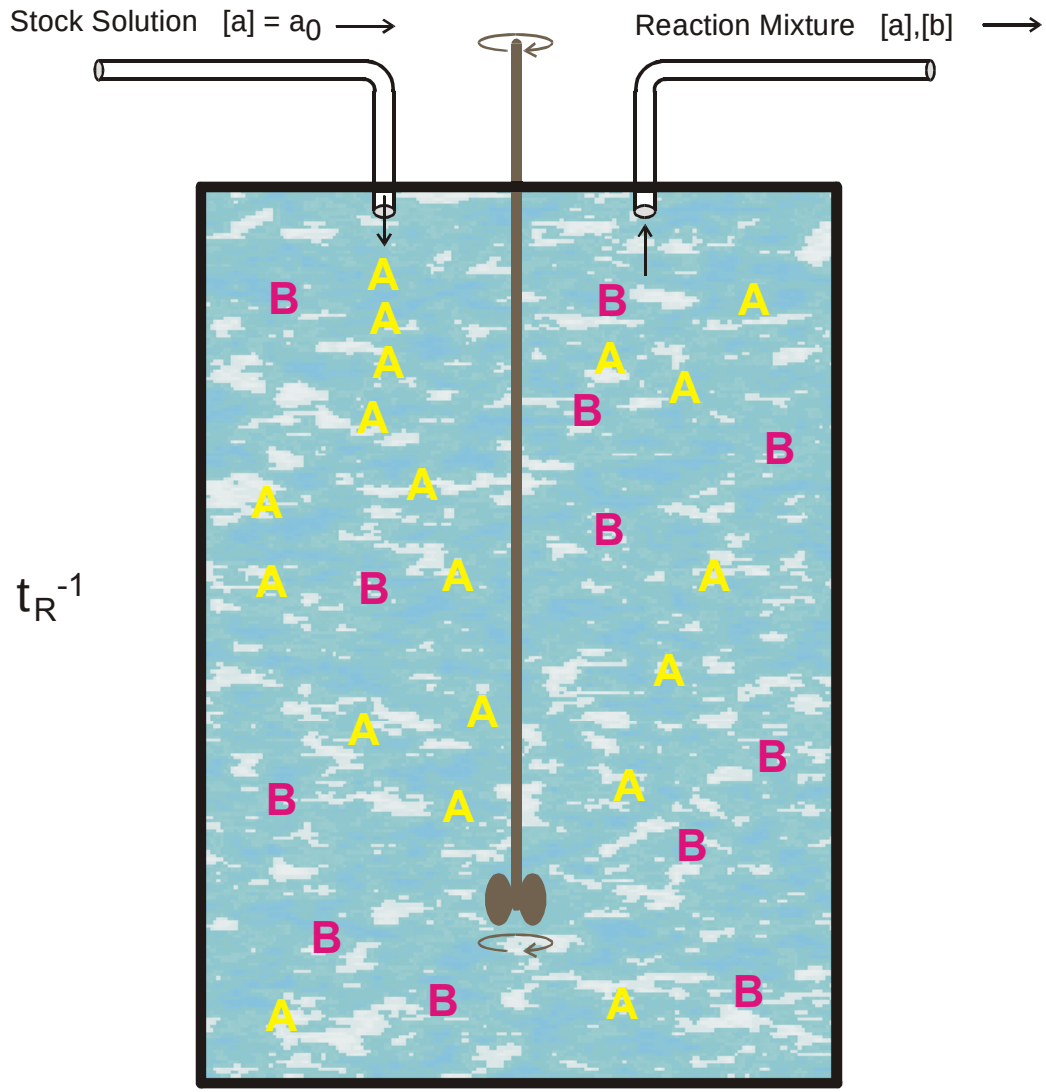
$d_iS \text{ Æ } 0$

Entropy changes in different thermodynamic systems

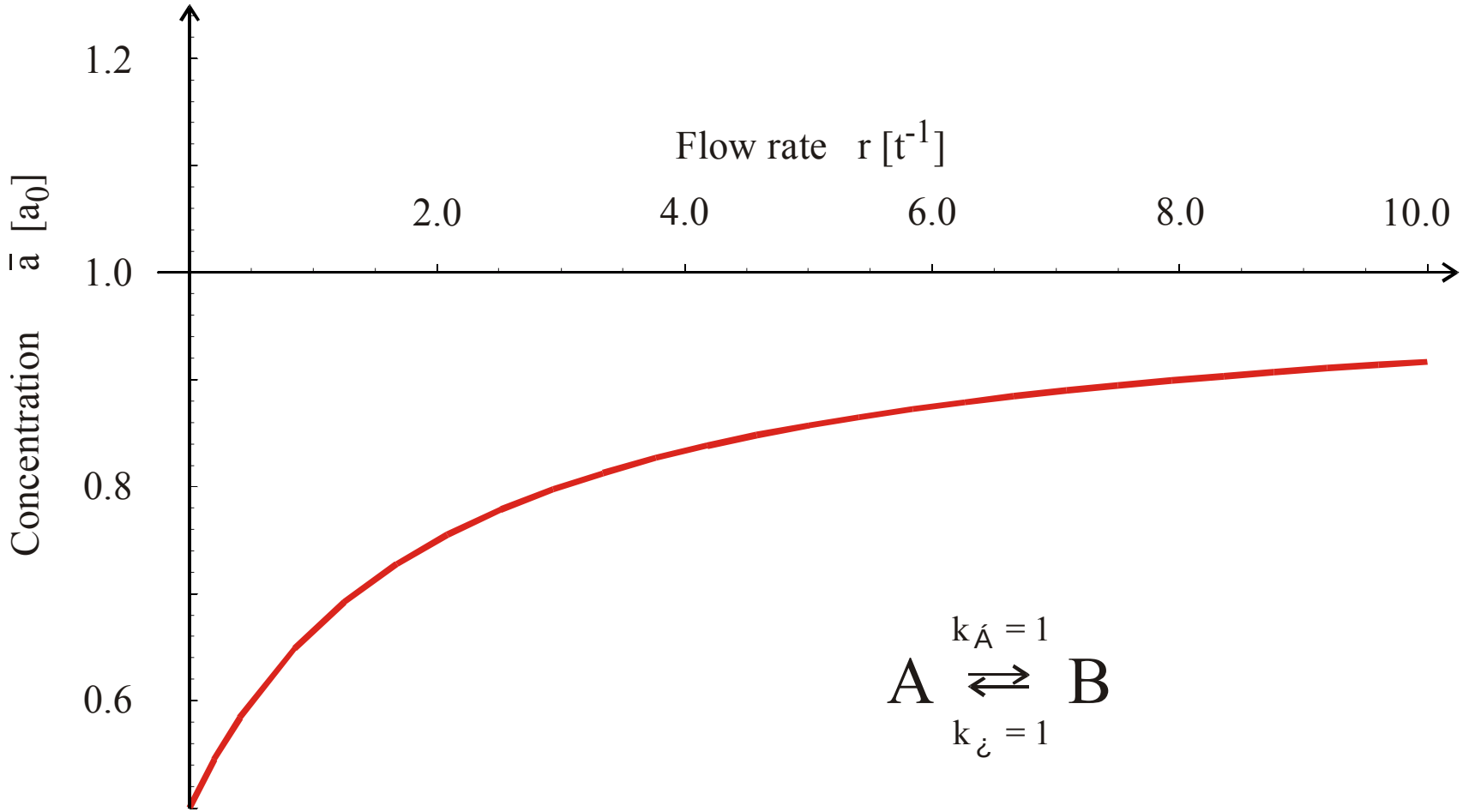
* Á A
A Á B
A Á Ø

B Á A
B Á Ø

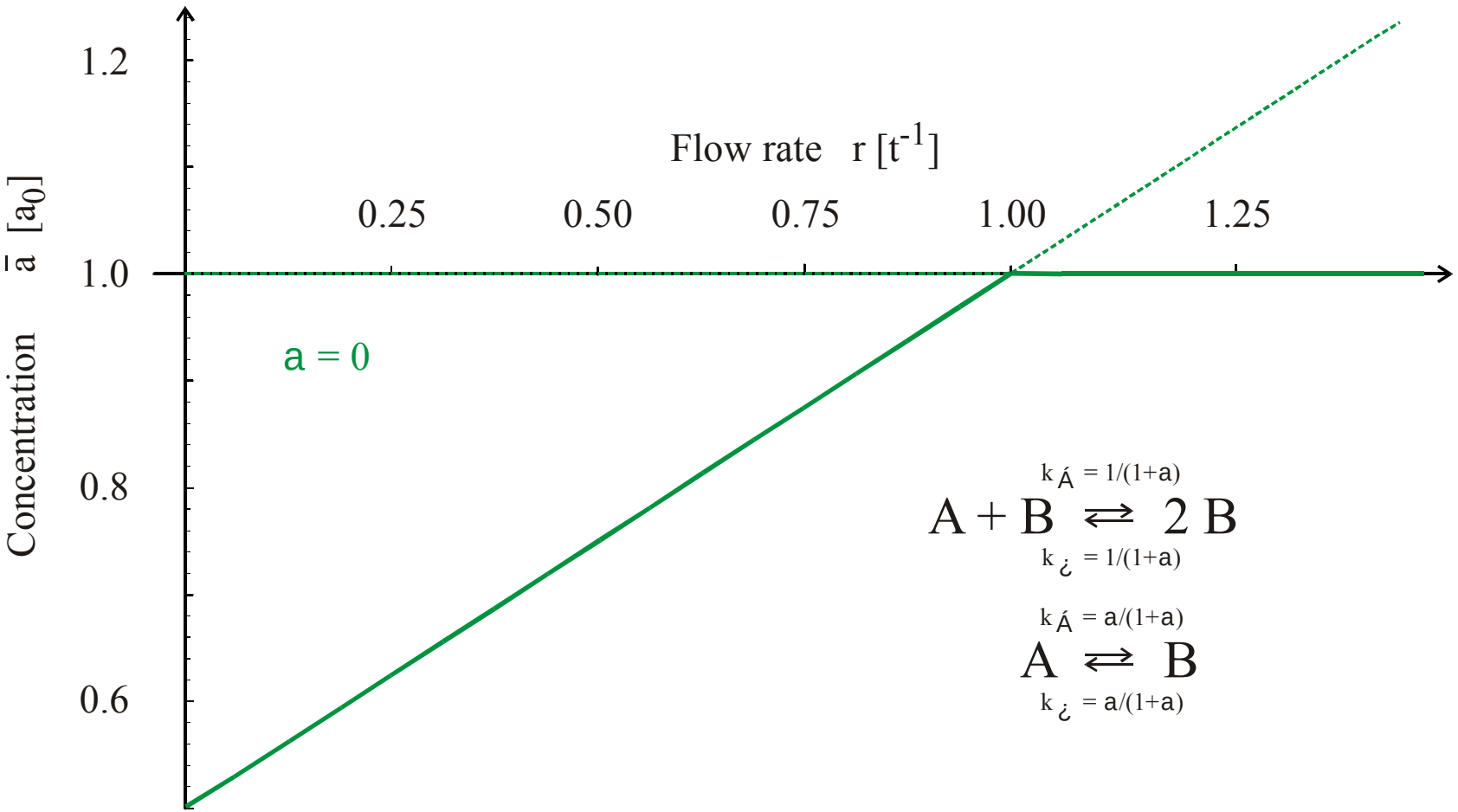
Flow rate $r = t_R^{-1}$



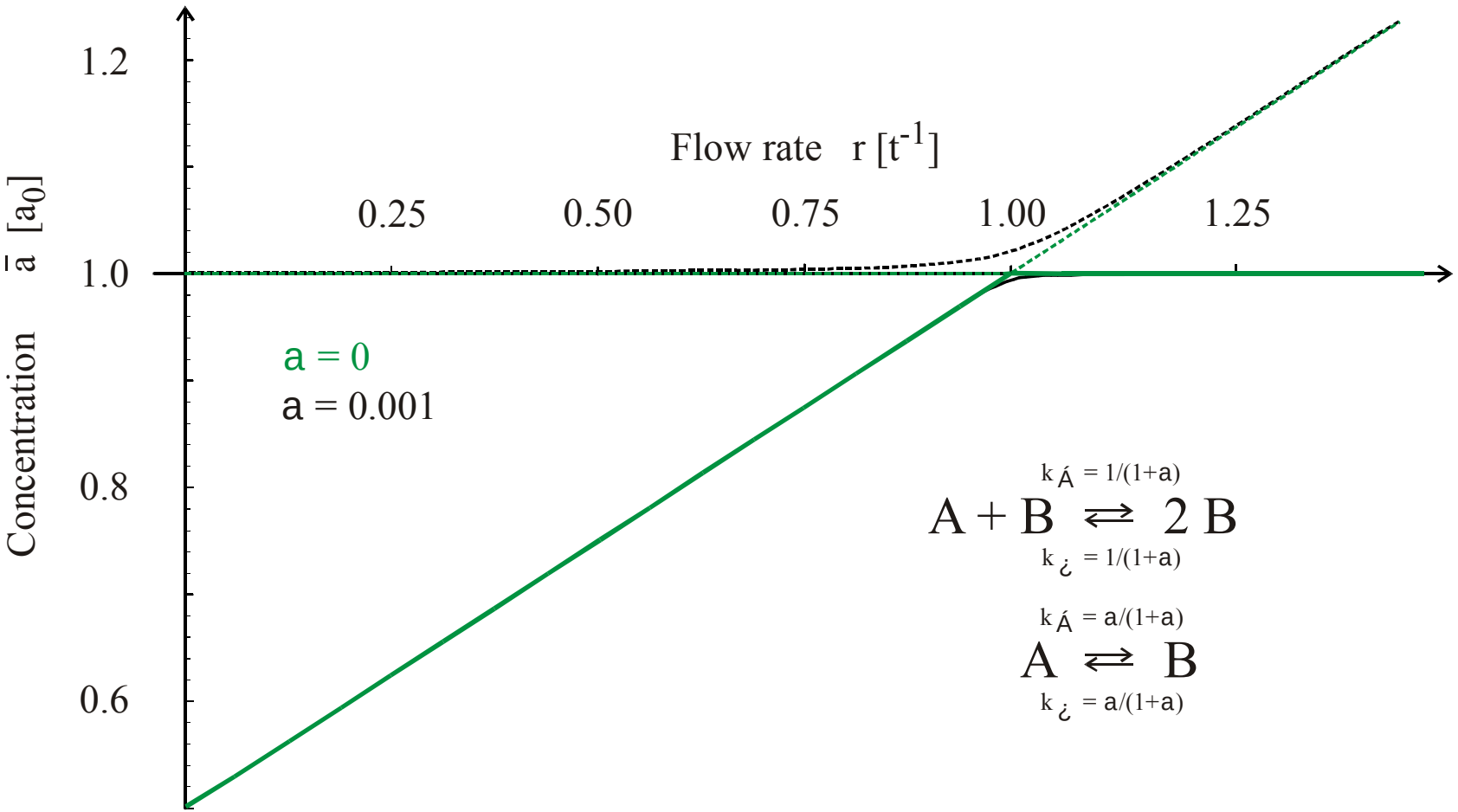
Reactions in the continuously stirred tank reactor (CSTR)



Reversible first order reaction in the flow reactor



Autocatalytic second order reaction and uncatalyzed reaction in the flow reactor



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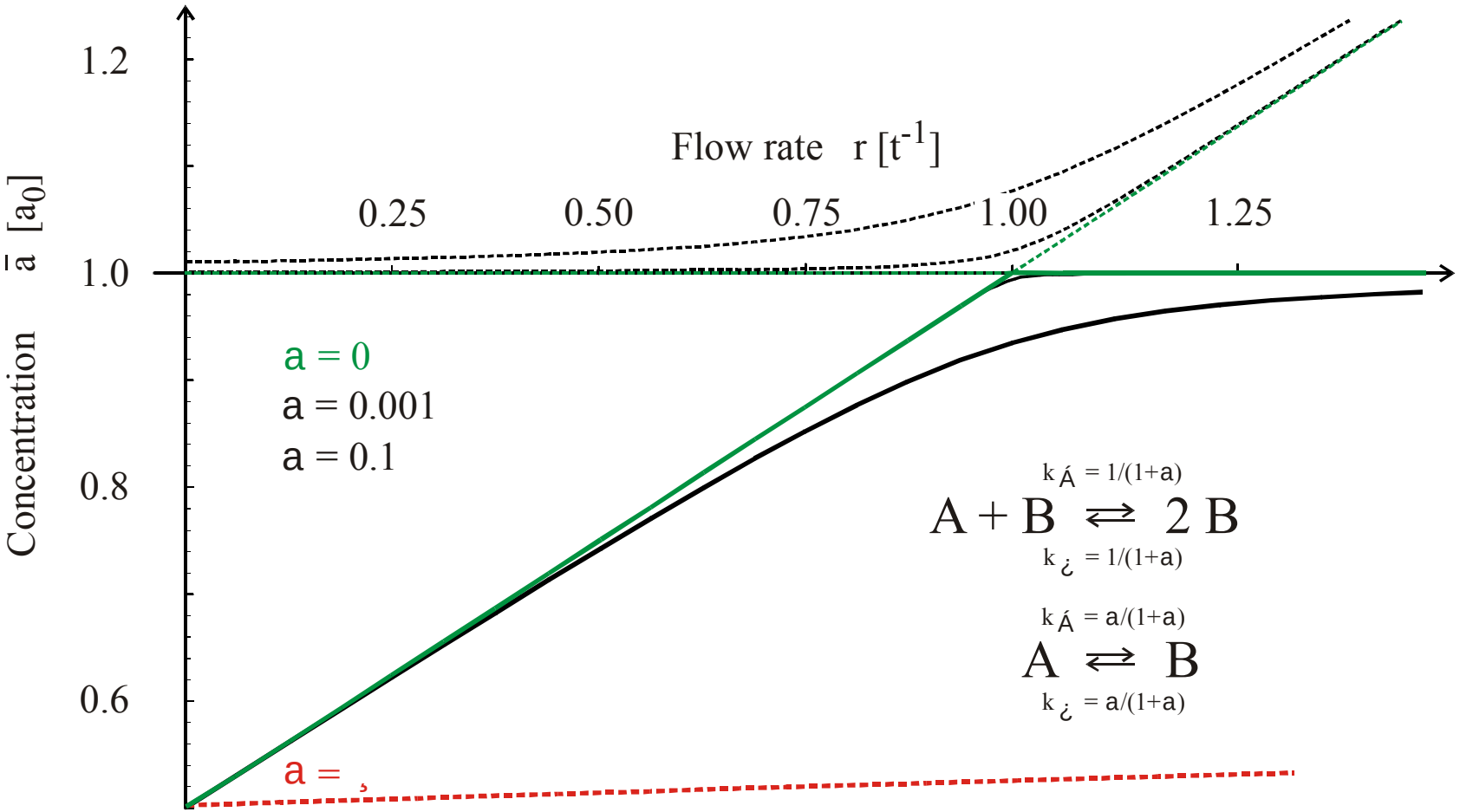

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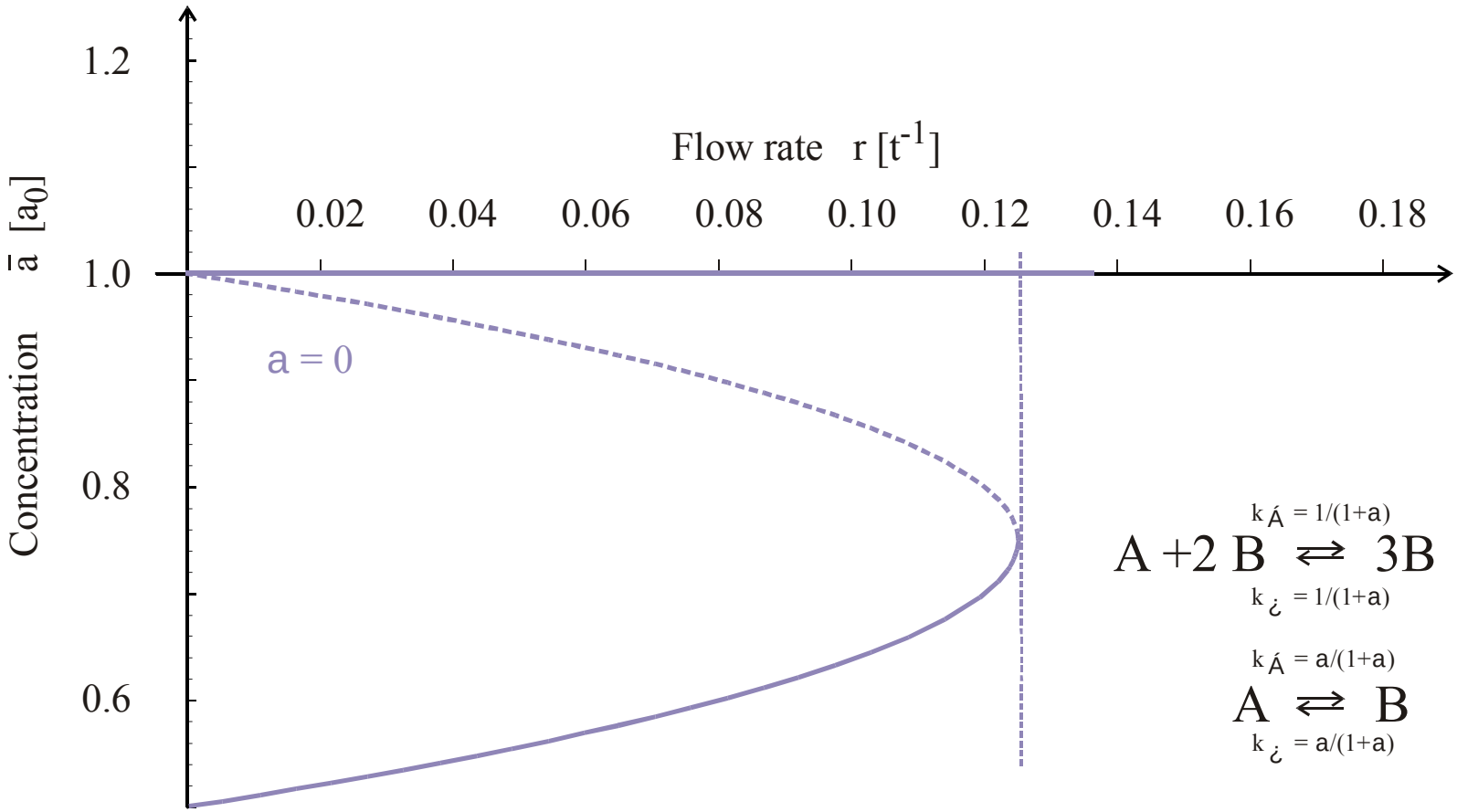
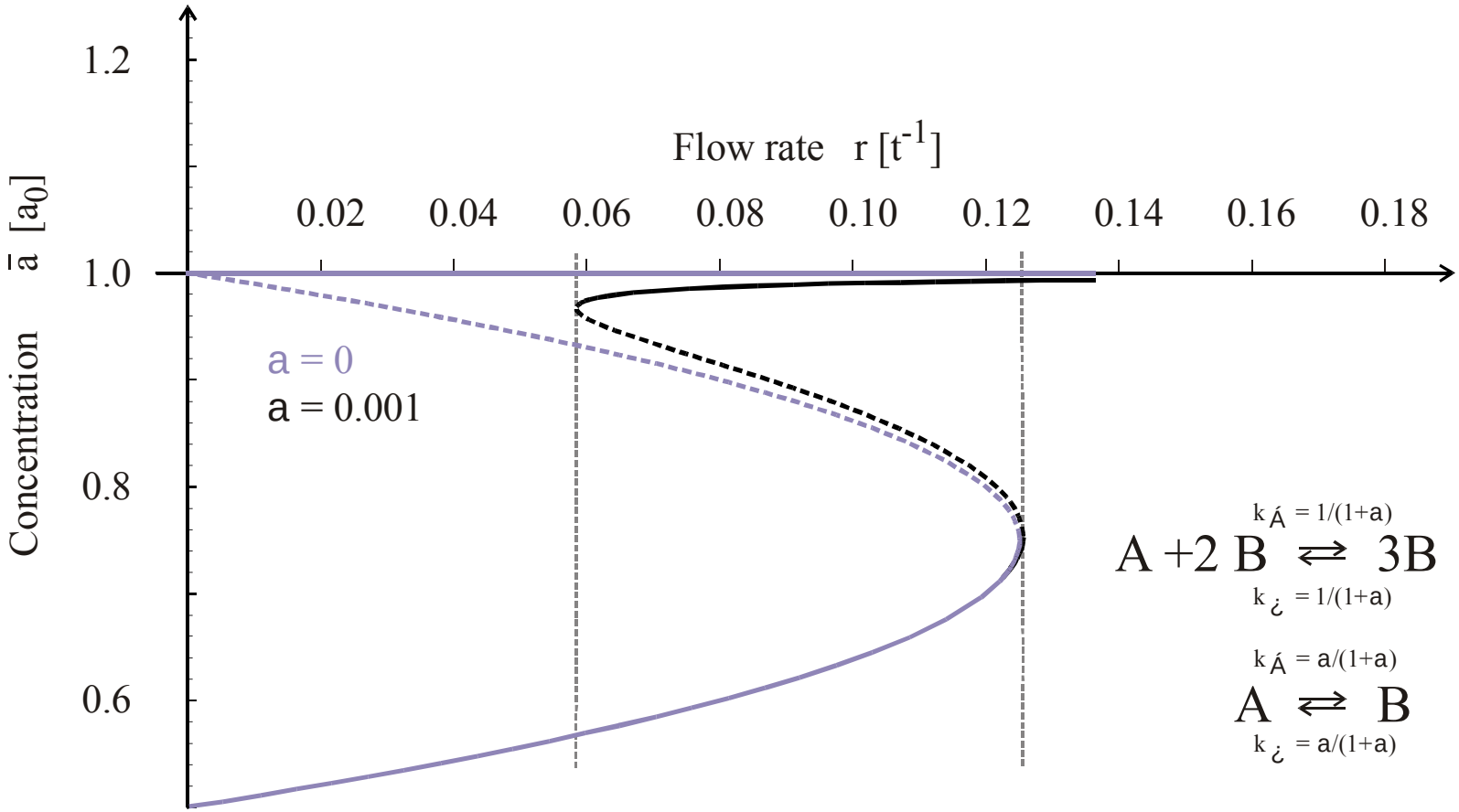


Autocatalytic third order reaction and uncatalyzed reaction in the flow reactor



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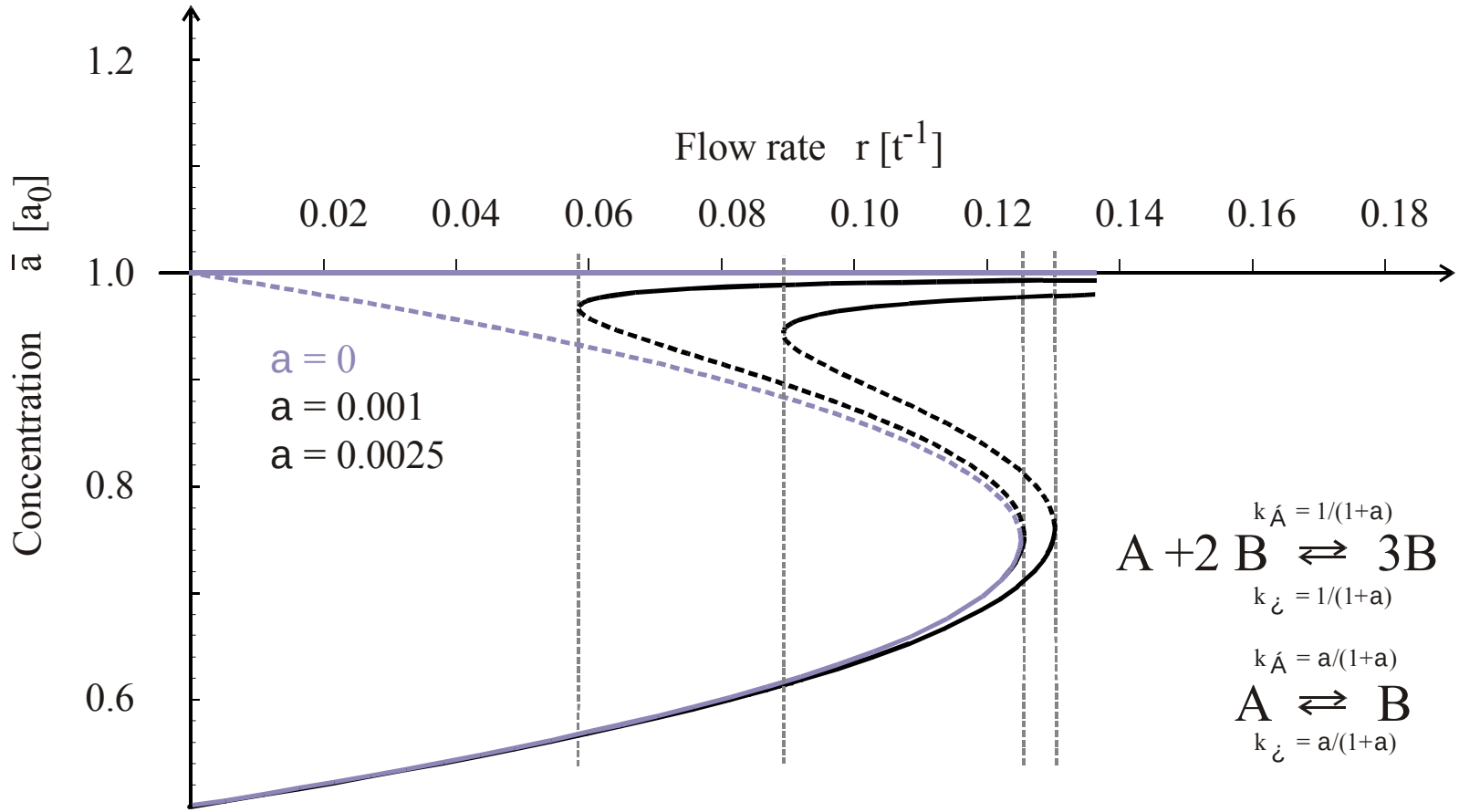

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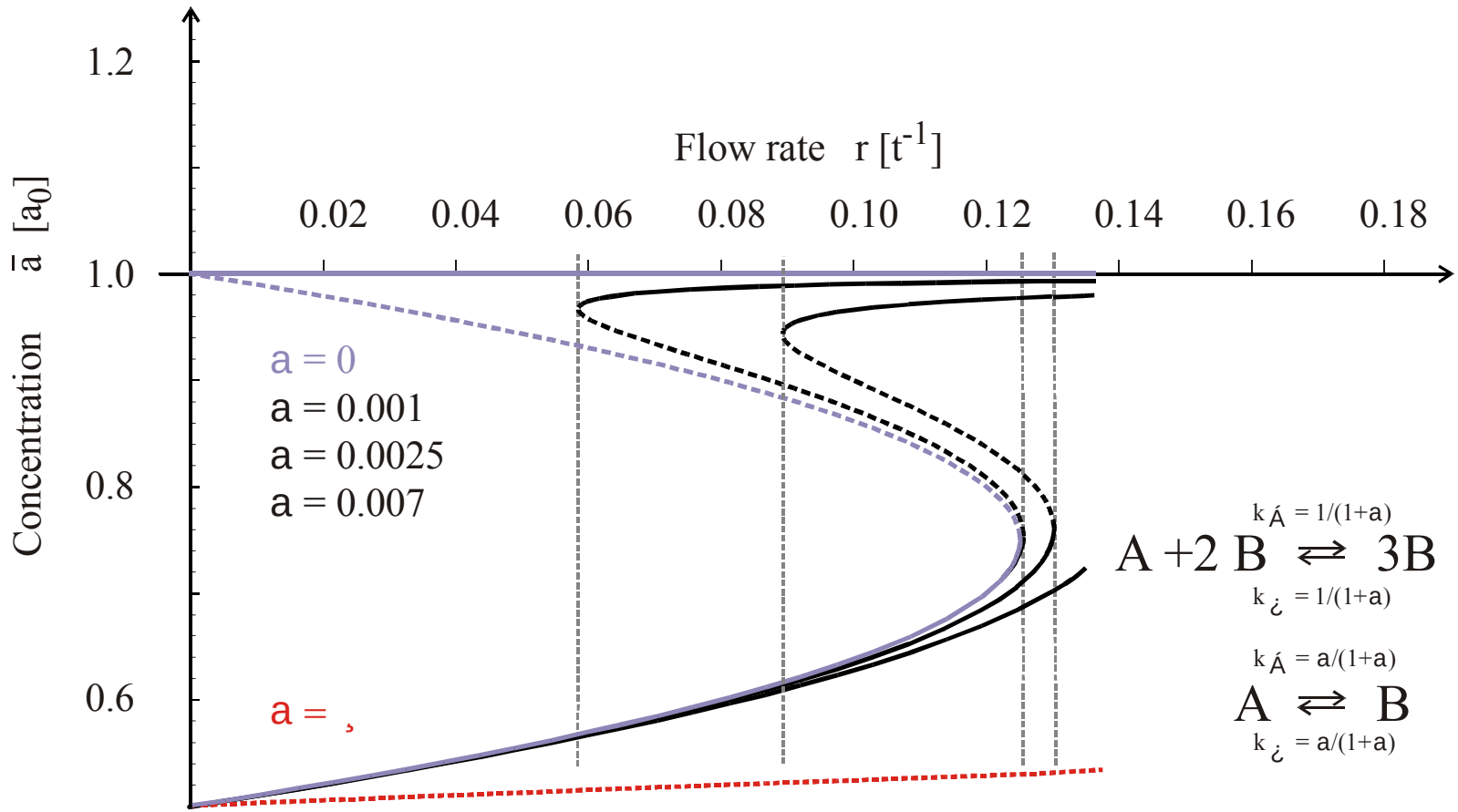
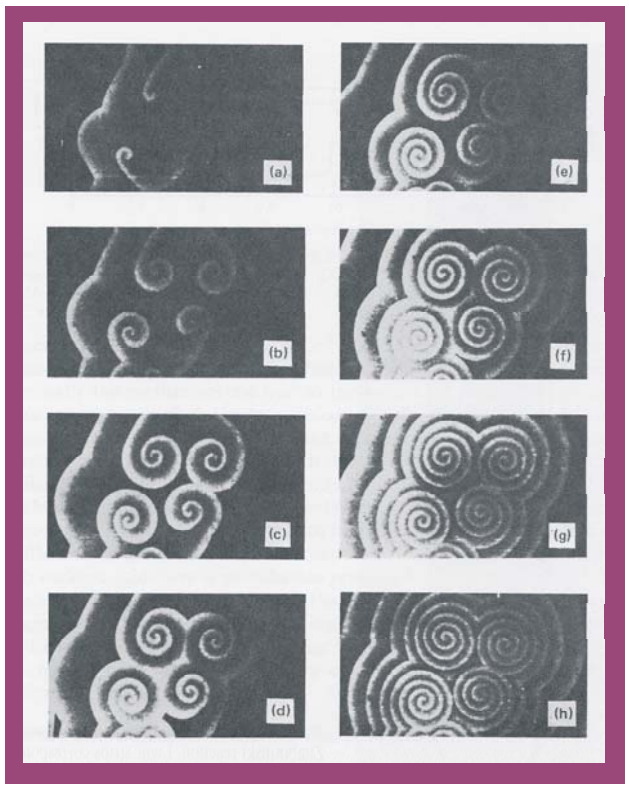


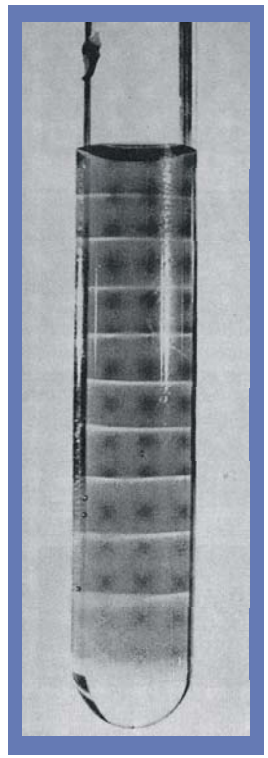
Autocatalytic third order reaction and uncatalyzed reaction in the flow reactor

Autocatalytic third order reactions

Direct, $A + 2X \rightarrow 3X$, or hidden in the reaction mechanism (Belousow-Zhabotinskii reaction).

- Multiple steady states
- Oscillations in homogeneous solution
- Deterministic chaos
- Turing patterns
- Spatiotemporal patterns (spirals)
  - Deterministic chaos in space and time



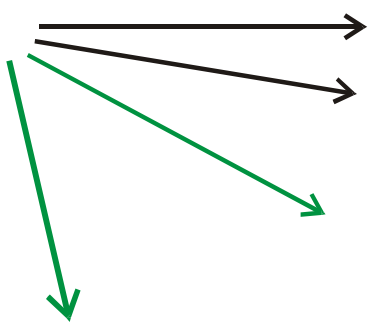


Pattern formation in autocatalytic third order reactions

G.Nicolis, I.Prigogine. *Self-Organization in Nonequilibrium Systems. From Dissipative Structures to Order through Fluctuations*. John Wiley, New York 1977

Autocatalytic second order reactions

Direct, **A + I Á 2 I** , or hidden in the reaction mechanism



Chemical self-enhancement

Combustion and chemistry of flames

Selection of laser modes

Selection of molecular or organismic species competing for common sources

Autocatalytic second order reaction as basis for selection processes.

The autocatalytic step is formally equivalent to replication or reproduction.

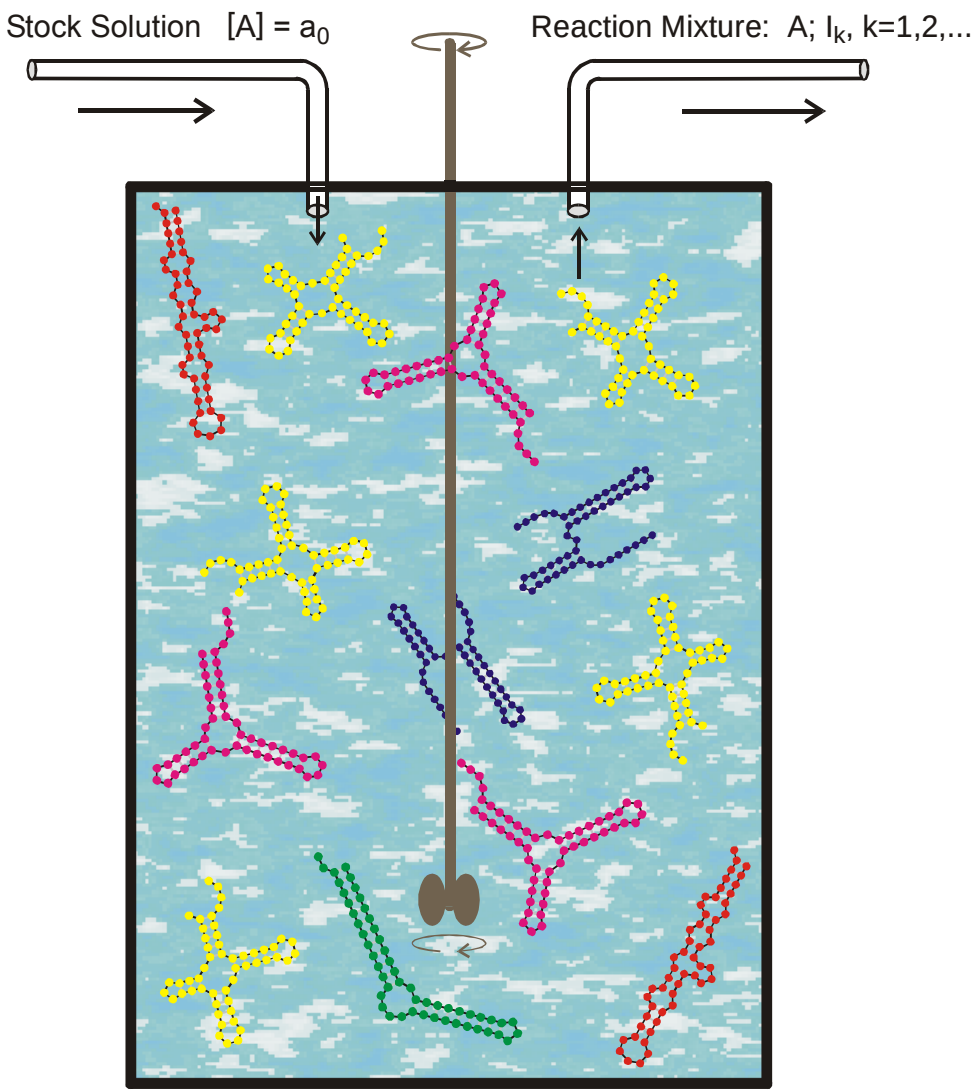
$$A + I_1 \underset{d_1}{\overset{k_1}{\rightleftharpoons}} 2\,I_1$$

$$A + I_2 \underset{d_2}{\overset{k_2}{\rightleftharpoons}} 2\,I_2$$

$$A + I_3 \underset{d_3}{\overset{k_3}{\rightleftharpoons}} 2\,I_3$$

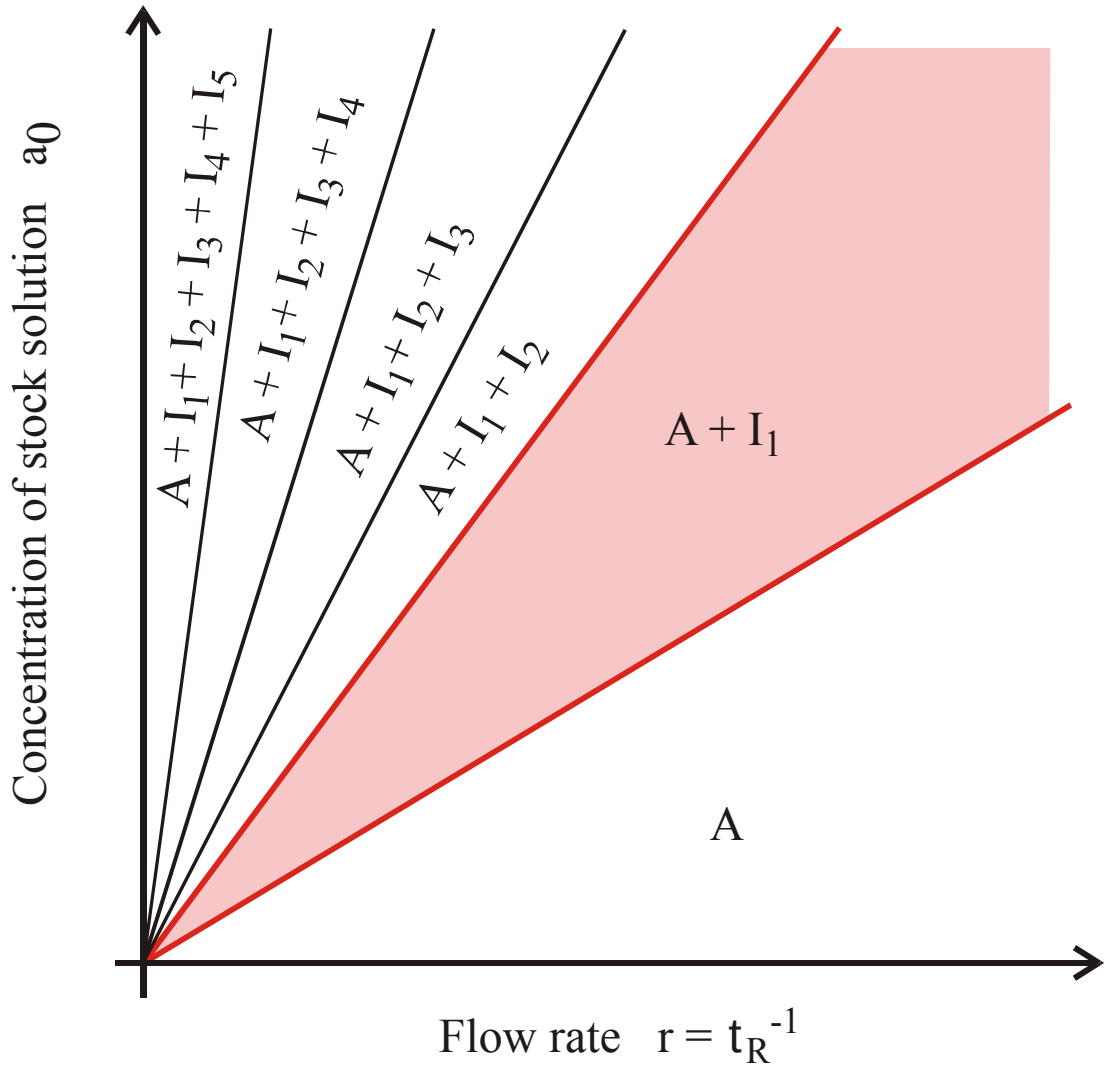
$$A + I_4 \underset{d_4}{\overset{k_4}{\rightleftharpoons}} 2\,I_4$$

$$A + I_5 \underset{d_5}{\overset{k_5}{\rightleftharpoons}} 2\,I_5$$



Autocatalytic competition in the flow reactor

P.Schuster & K.Sigmund, Dynamics of evolutionary optimization, *Ber.Bunsenges.Phys.Chem.* **89**: 668-682 (1985)



$$A + I_1 \rightleftarrows 2\,I_1$$

$$A + I_2 \rightleftarrows 2\,I_2$$

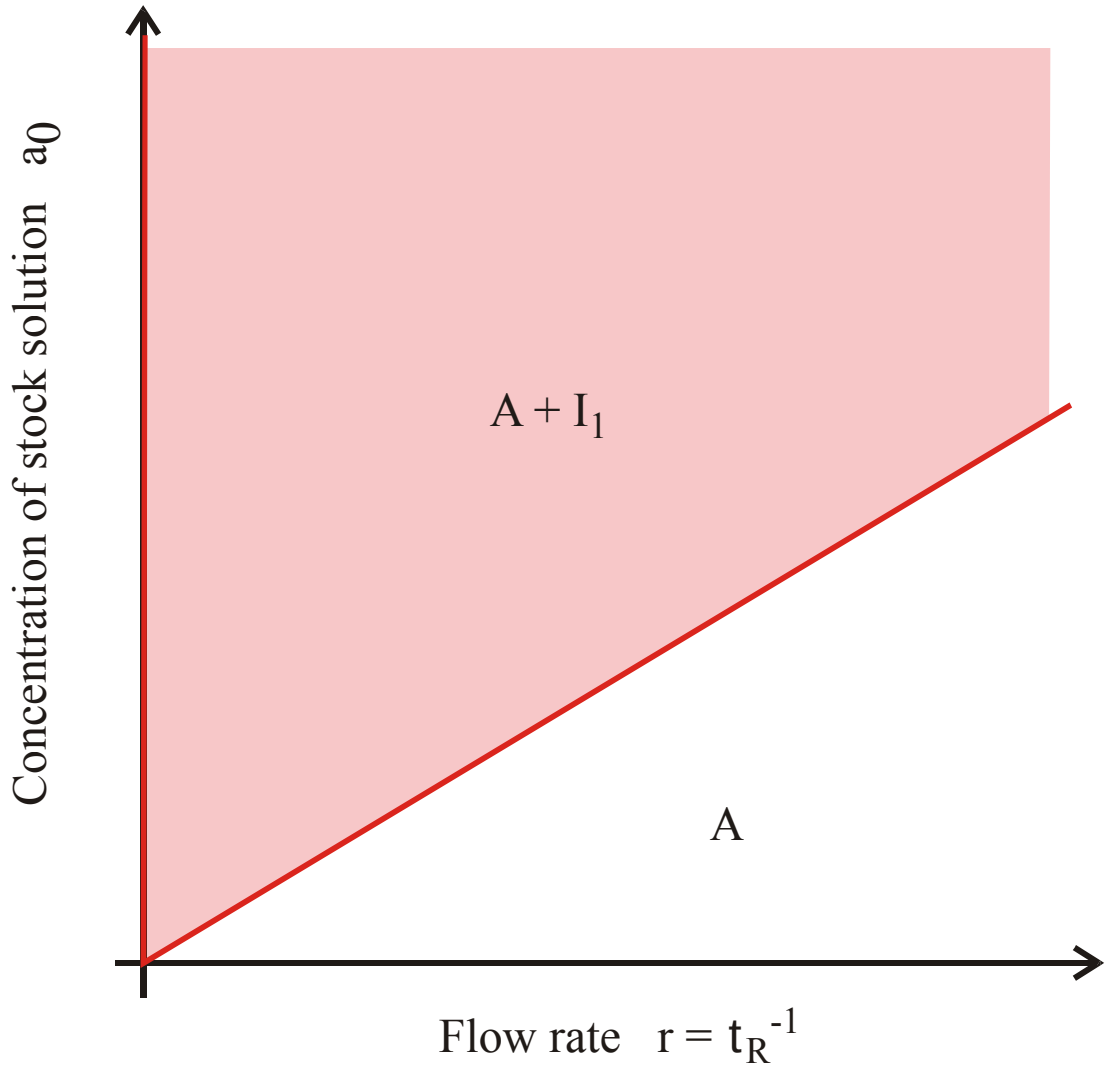
$$A + I_3 \rightleftarrows 2\,I_3$$

$$A + I_4 \rightleftarrows 2\,I_4$$

$$A + I_5 \rightleftarrows 2\,I_5$$

$$k_1 > k_2 > k_3 > k_4 > k_5$$

Selection in the flow reactor: Reversible replication reactions



$$A + I_1 \longrightarrow 2\,I_1$$

$$A + I_2 \longrightarrow 2\,I_2$$

$$A + I_3 \longrightarrow 2\,I_3$$

$$A + I_4 \longrightarrow 2\,I_4$$

$$A + I_5 \longrightarrow 2\,I_5$$

$$k_1 > k_2 > k_3 > k_4 > k_5$$

Selection in the flow reactor: Irreversible replication reactions

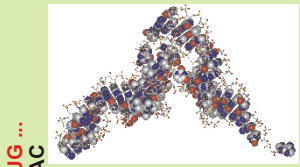
RNA

RNA *as transmitter of genetic information*

DNA
↓ transcription
...AGAGCGCCAGACUGAAGAUCUGGAGGUCCUGUGUUC...
messenger-RNA
↓ translation
protein

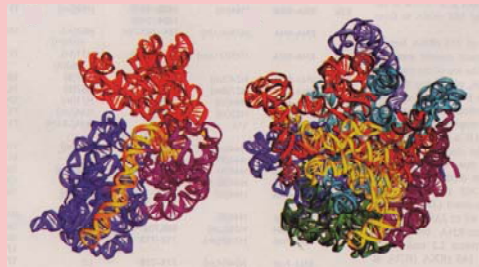
RNA as **working copy** of genetic information

RNA *as adapter molecule*



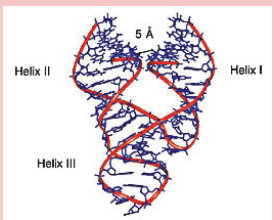
genetic code

RNA *is the catalytic subunit in supramolecular complexes*



The ribosome is a ribozyme !

RNA *as catalyst*



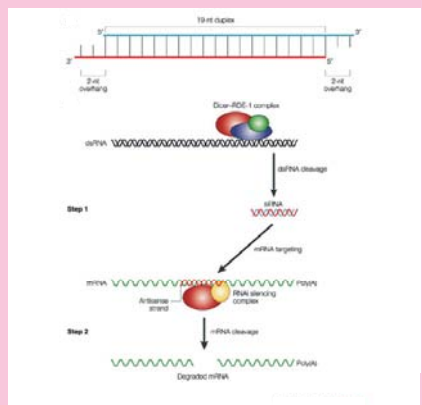
ribozyme

RNA *is modified by epigenetic control*

RNA editing

Alternative splicing of messenger RNA

RNA *as regulator of gene expression*



gene silencing by small interfering RNAs

RNA *as carrier of genetic information*

RNA viruses and retroviruses

RNA as information carrier in evolution *in vitro* and evolutionary biotechnology

The RNA *world as a precursor of the current* DNA + protein *biology*

Functions of RNA molecules