Navigating the crossroads between chemistry and mathematics – how much is actually “just maths”?

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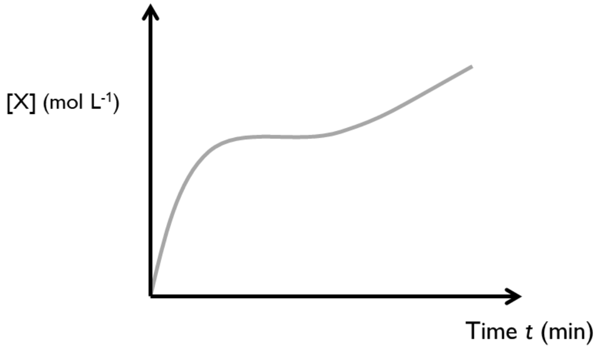
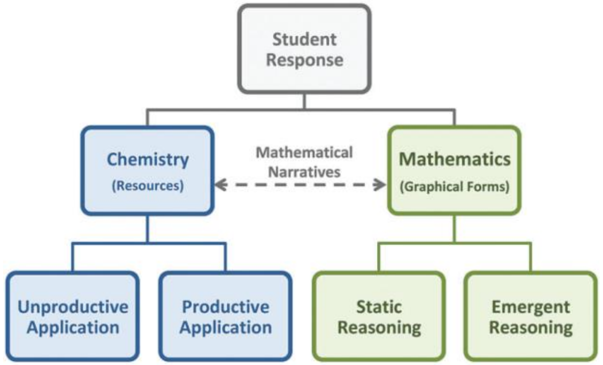
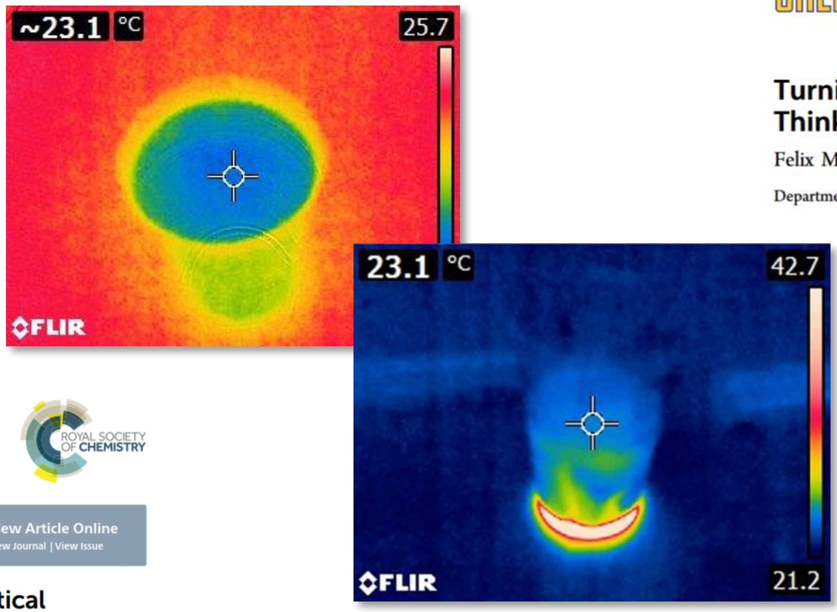
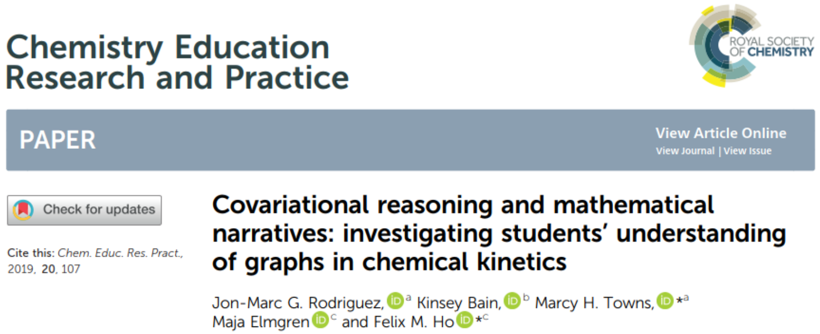
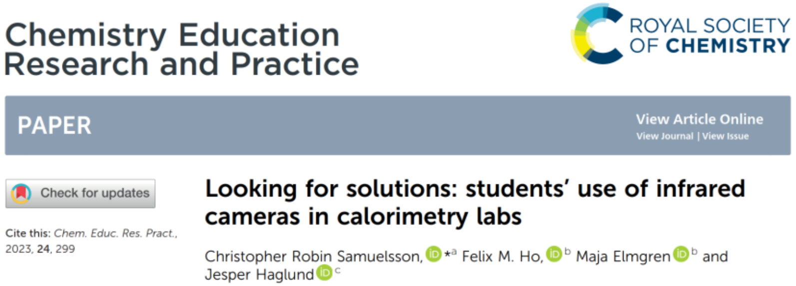
- Crossroads between chemistry and mathematics
- Systems thinking
- IR-cameras in chemistry teaching











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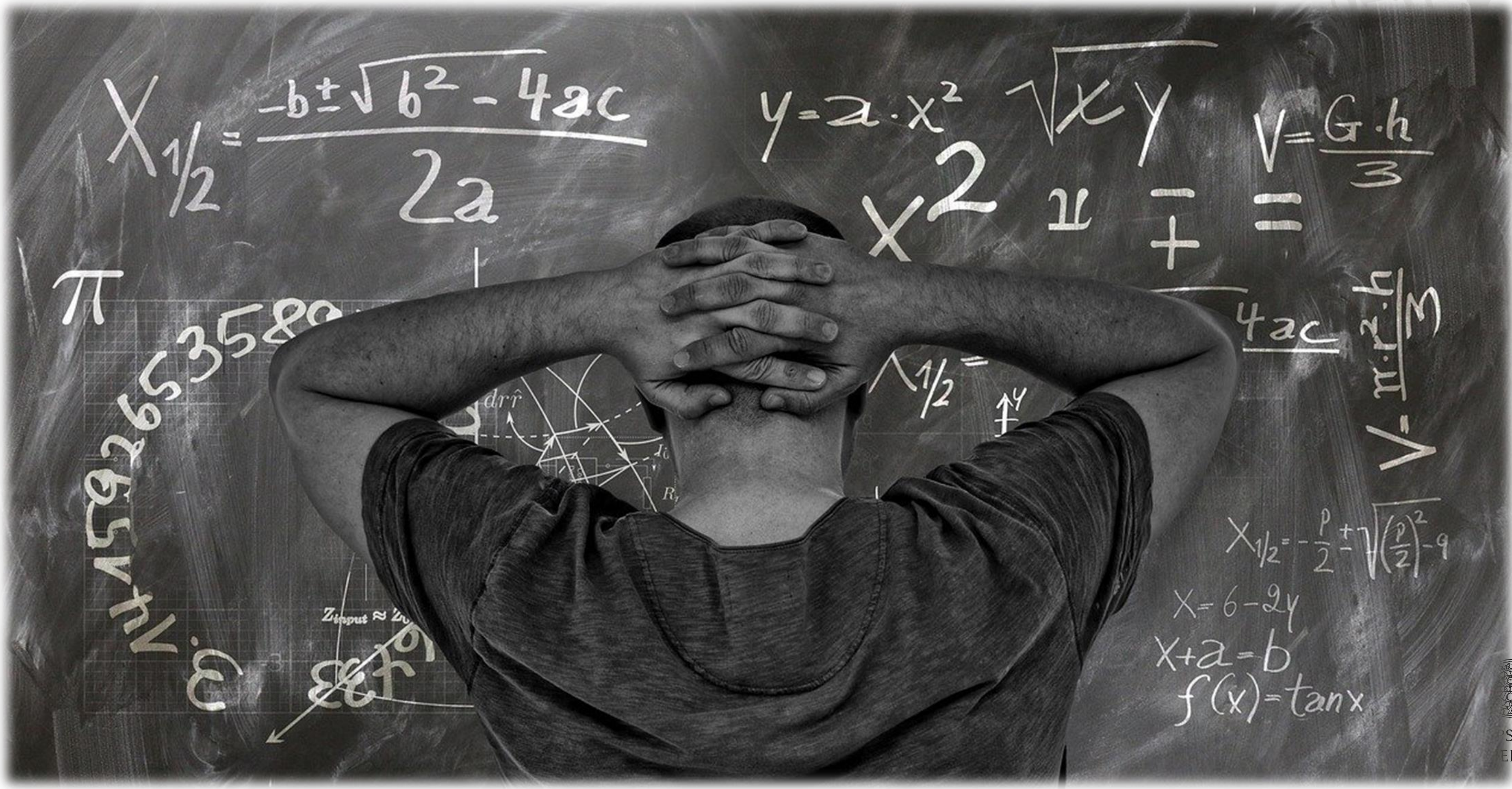
”Students just can’t do maths”

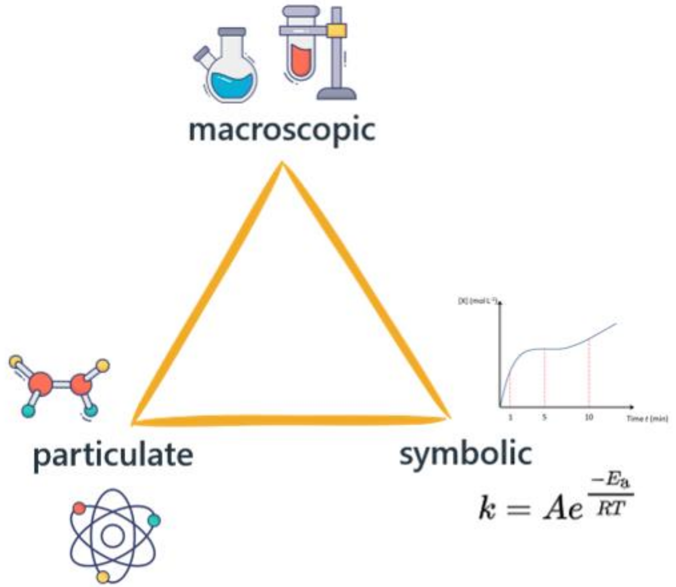


Why does it matter?

- Mathematics is part of the language of chemistry, also for tool for analysis and modelling.
  e.g. Towns, Bain & Rodriguez (eds, 2019); Johnstone (1991, 2009)

- Documented difficulties chemistry students have with mathematics.
  Algorithmic, ”plug-and-chug” *vs.* conceptual understanding
  e.g. Camacho & Good (1989); Potgieter et al, 2008; Chandrasegaran et al (2009); Becker & Towns (2012)

- Thinking with models vs. thinking about models
  Schwarz et al (2016), Winschitl et al (2008), Lazenby & Becker (2019)



Why does it matter?

- Pinpointing where support is (additionally) needed
  - E.g. in remedial / preparatory courses
- Framework for designing instruction and support

- Still under-researched, especially at the HE level; much room for collaboration across DBER fields.

  e.g. Towns, Bain & Rodriguez (eds, 2019); Bain et al (2019)

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How can we study the interactions between chemistry and mathematics?

What kind of interactions?

Where can we find them?

How would we characterise and classify them?

What processes are involved?

What do we mean by maths and ”doing maths”?

The ”anti-cliffhanger”

- It’s much more than teaching and learning the ”right” maths and the ”right” chemistry
    - there are many more factors at play than content in the learning and using mathematics contextualised in other disciplines
- There are numerous issues concerning aims and goals for teaching and learning that effect the answer to how mathematics education in/for other disciplines should be approached

Ye *et al*, *Chemistry Education Research and Practice* (2024), **25**, 242 - 265

Student problem-solving in chemical kinetics

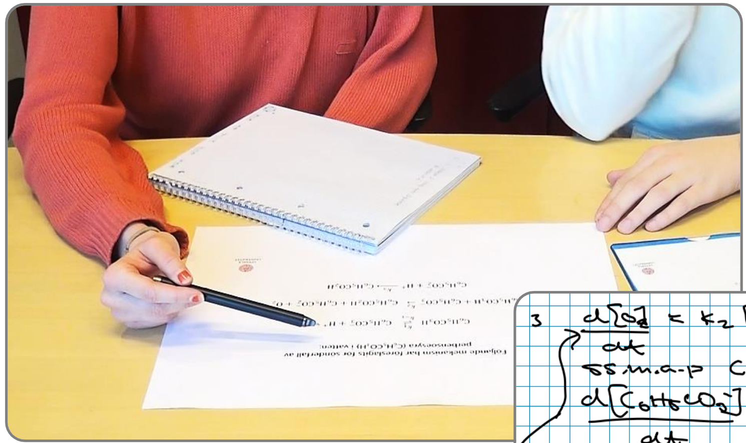
The following mechanism has been proposed for the decomposition of perbenzoic acid ($C_6H_5CO_3H$) in water:

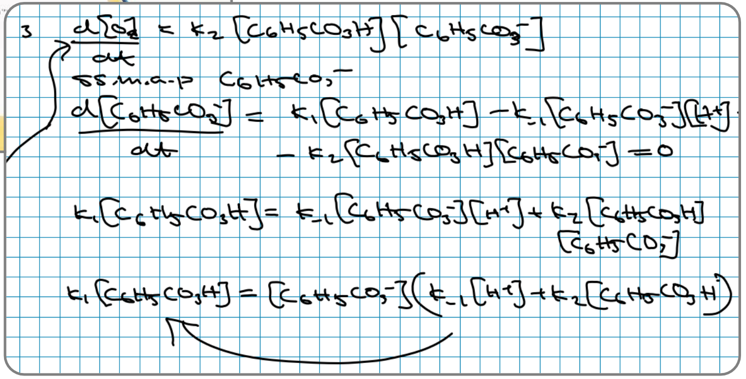
$$C_6H_5CO_3H \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C_6H_5CO_3^- + H^+$$

$$C_6H_5CO_3H + C_6H_5CO_3^- \xrightarrow{k_2} C_6H_5CO_2H + C_6H_5CO_2^- + O_2$$

$$C_6H_5CO_2^- + H^+ \xrightarrow{k_3} C_6H_5CO_2H$$

Derive an expression for the **rate of formation of O_2**. Assume that the steady-state approximation is applicable. Explain your thinking out loud.





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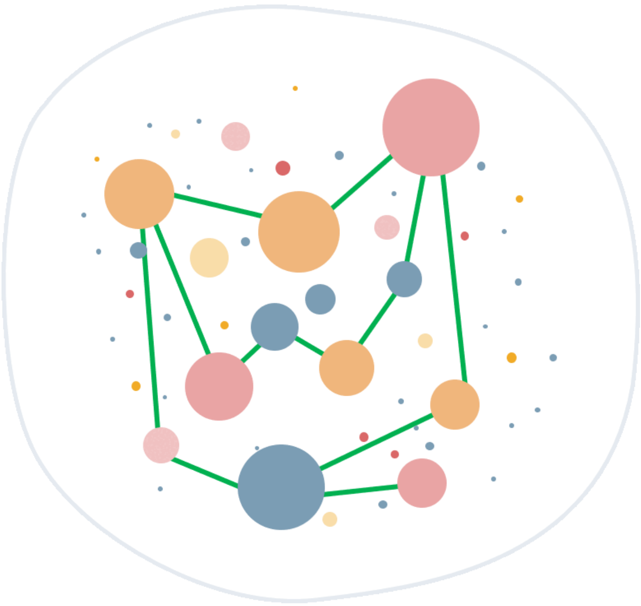
Resource framework & epistemological framing

Knowledge is constructed from small cognitive units **(resources)** connected in **dynamic networks**.

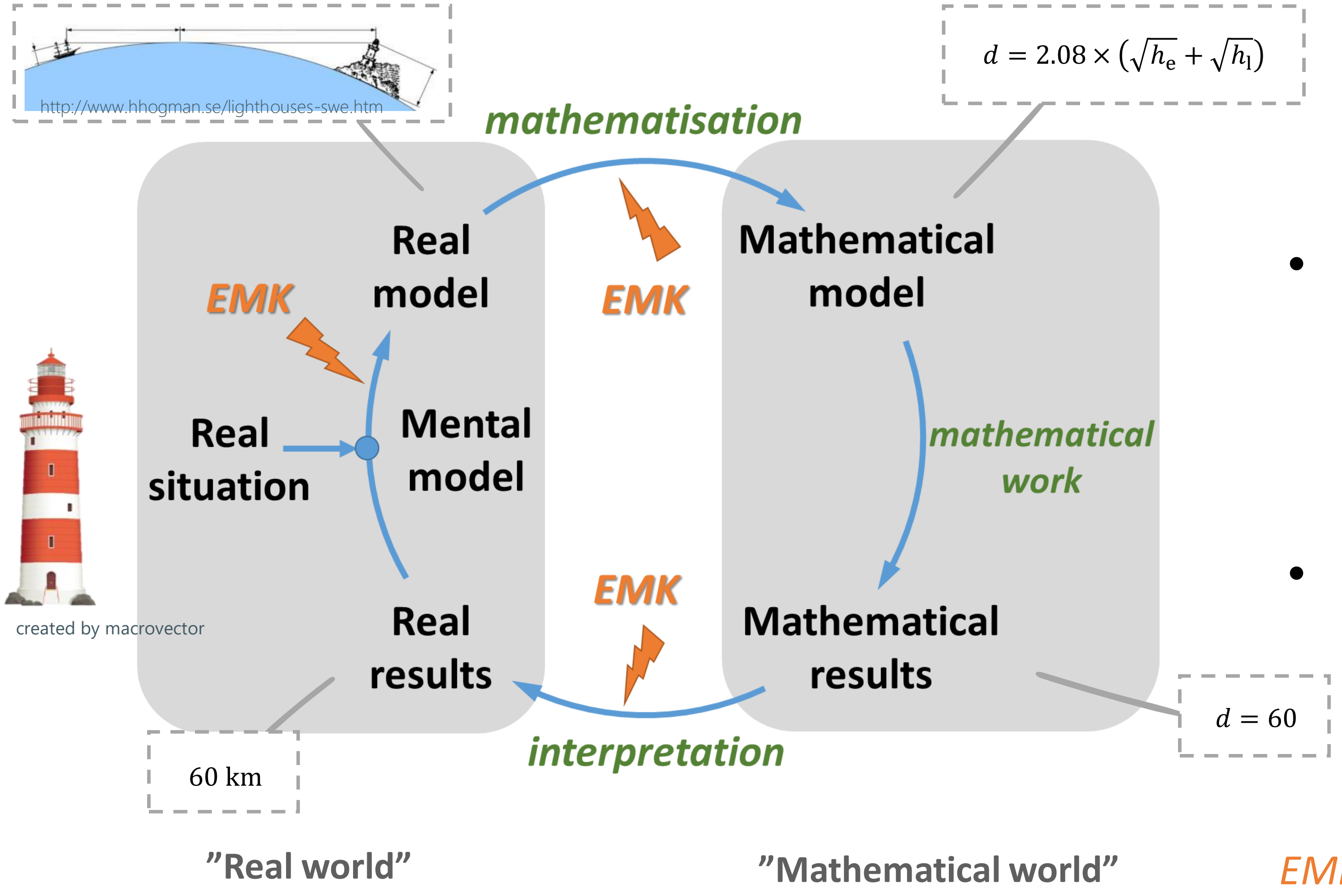
What resources that are **activated** depends on the **context (framing).**



See also the literature on transfer

Hammer & Elby (2002, 2003); Hammer, Elby, Scherr, & Redish (2005); Holme, Luxford, & Brandriet (2015)
See also Ivanjek (2016)

Mathematical Modelling Cycle (MMC)



Various versions have been proposed

- Idealised process, non-linear in reality, "bouncing around"
  e.g. Borromeo Ferri (2007); Lesh & Doerr (2012); Doerr et al (2017)
- Technical vs structural mathematics
  Pietrocola (2008); Uhden et al (2012)

EMK = extra mathematical knowledge

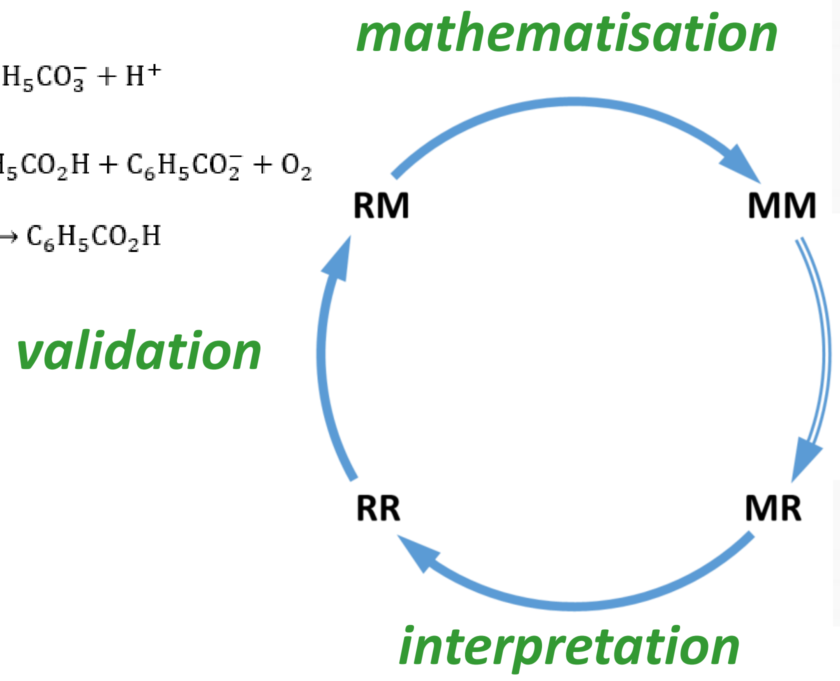
Adapted from Borromeo Ferri (2006); Blum & Leiß (2005).
See also: Doerr et al (2017), Ho et al (2019)

Where and how should we look?

$$C_6H_5CO_3H \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C_6H_5CO_3^- + H^+$$

$$C_6H_5CO_3H + C_6H_5CO_3^- \xrightarrow{k_2} C_6H_5CO_2H + C_6H_5CO_2^- + O_2$$

$$C_6H_5CO_2^- + H^+ \xrightarrow{k_3} C_6H_5CO_2H$$



$$\frac{d[O_2]}{dt} = k_2[C_6H_5CO_3H][C_6H_5CO_3^-]$$

$$\frac{d[C_6H_5CO_3^-]}{dt} = k_1[C_6H_5CO_3H] - k_{-1}[C_6H_5CO_3^-][H^+] - k_2[C_6H_5CO_3H][C_6H_5CO_3^-] \approx 0$$

$$\frac{d[O_2]}{dt} = \frac{k_1k_2[C_6H_5CO_3H]^2}{k_{-1}[H^+] + k_2[C_6H_5CO_3H]}$$

Non-mathematical realm

Mathematical realm

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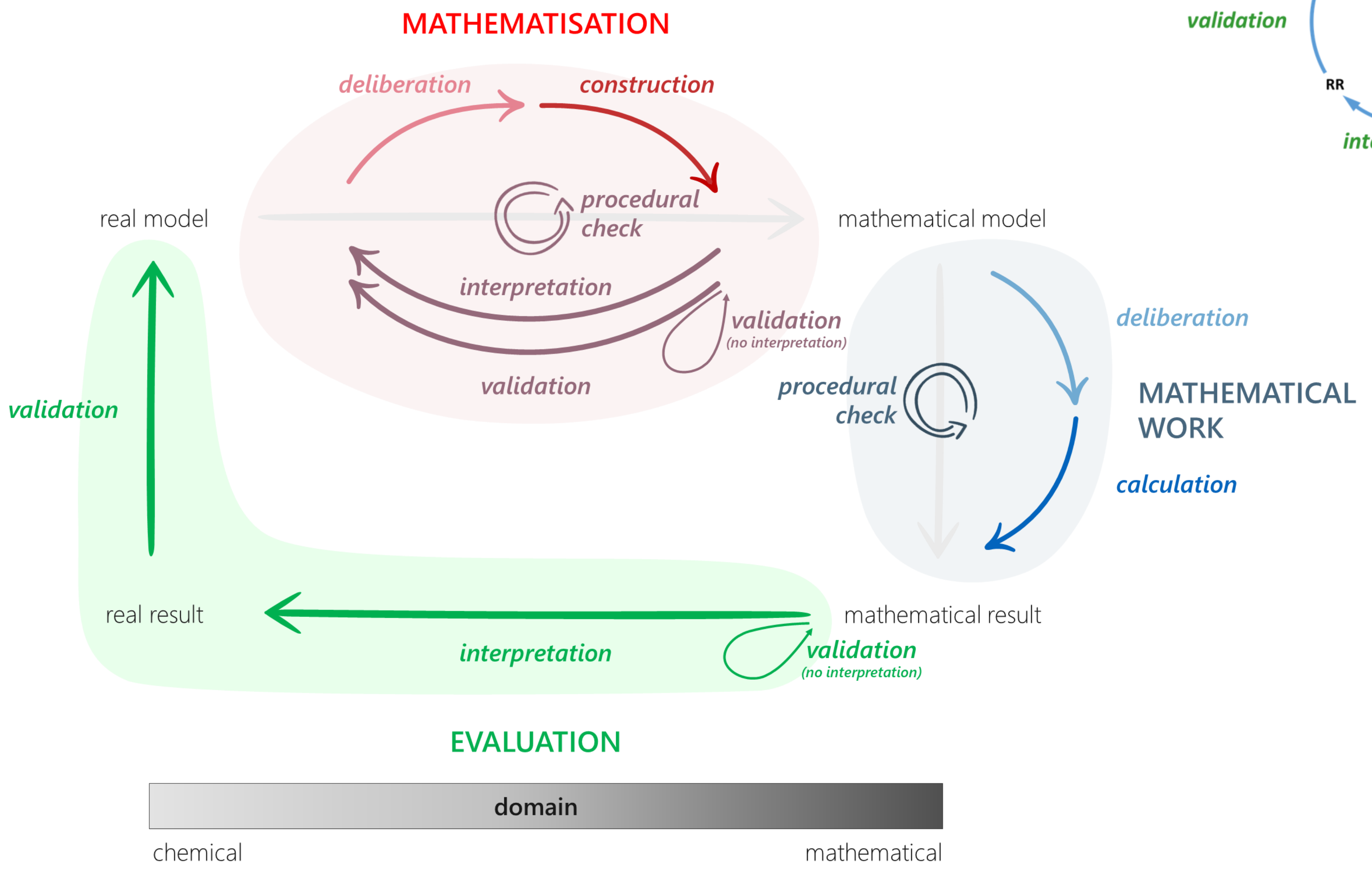
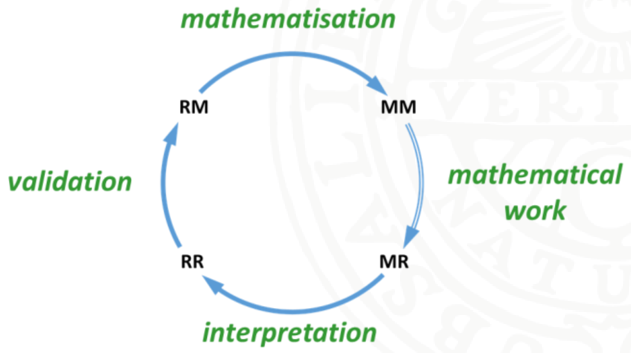
The extended MMC





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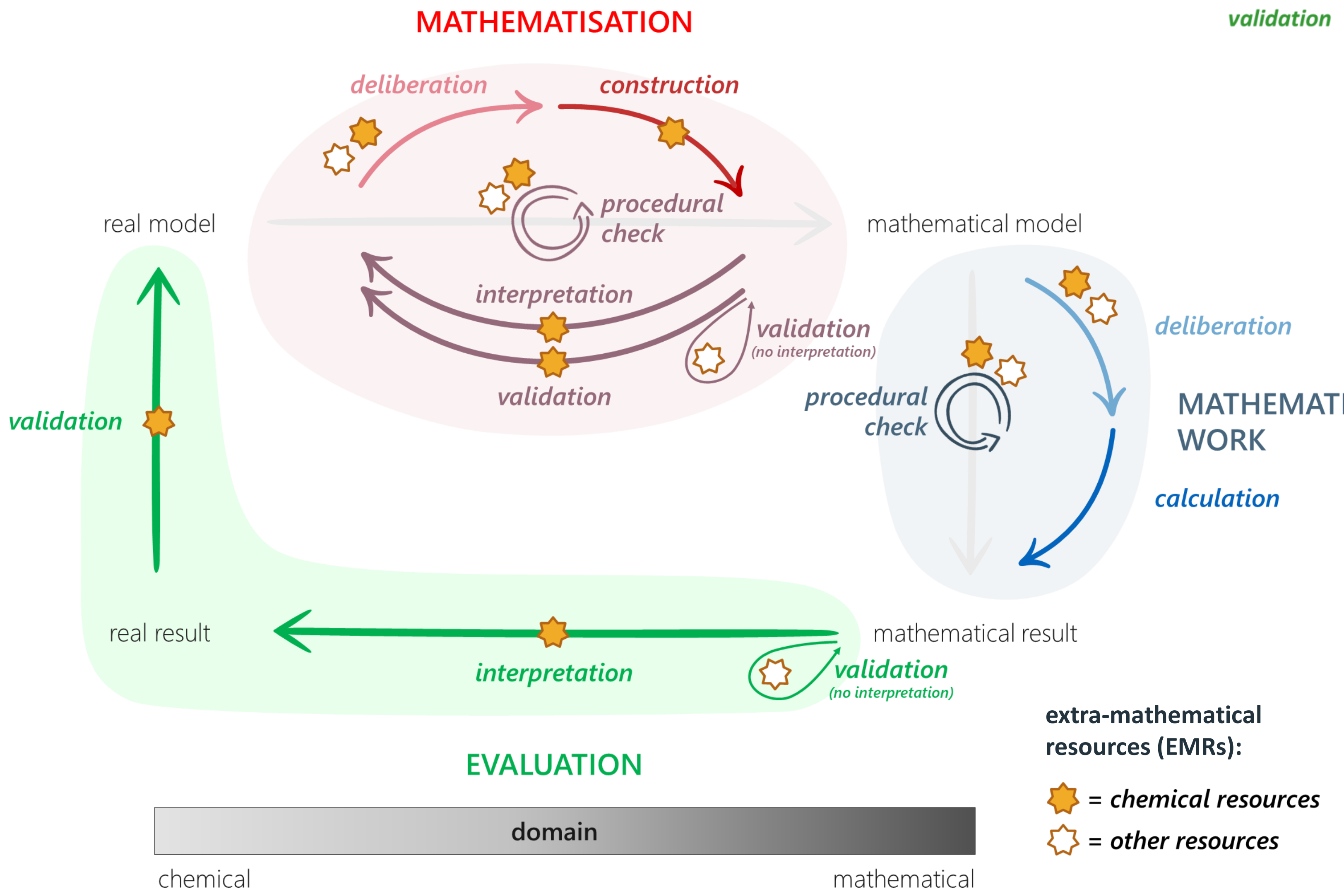
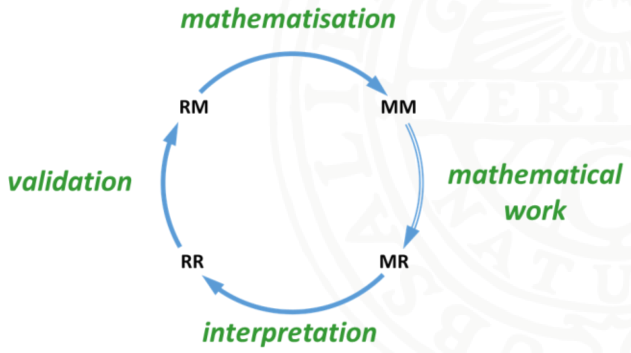
Ye *et al*, *Chemistry Education Research and Practice* (2024), **25**, 242 - 265

The extended MMC





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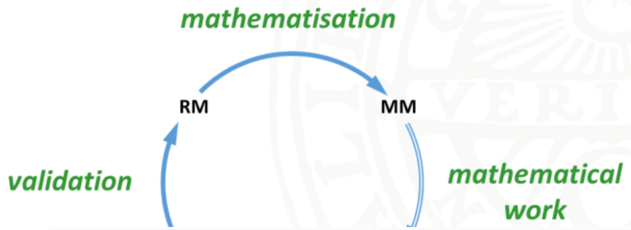
The extended MMC



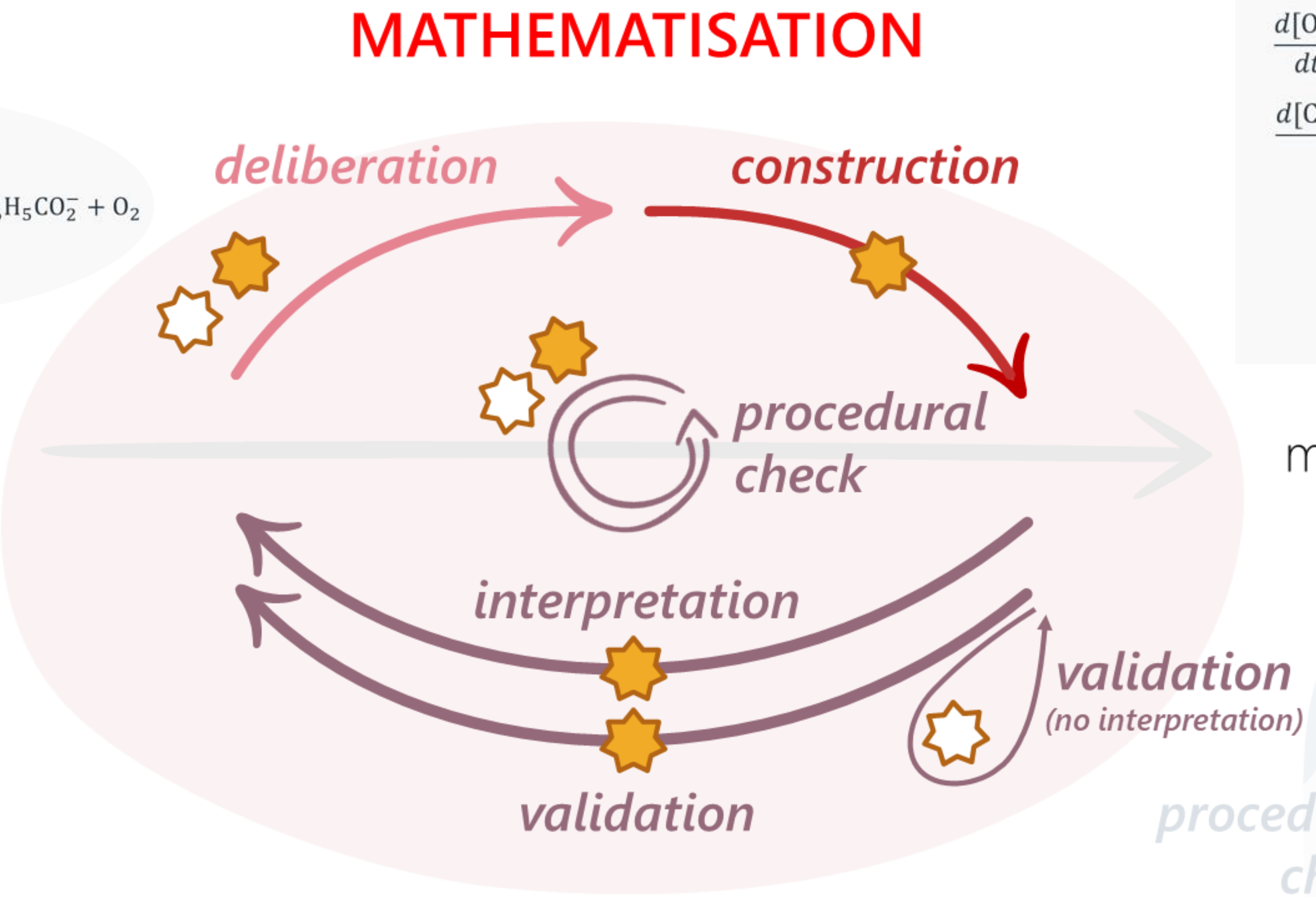
$$\frac{d[O_2]}{dt} = k_2[C_6H_5CO_3H][C_6H_5CO_3^-]$$

$$\frac{d[C_6H_5CO_3^-]}{dt} = k_1[C_6H_5CO_3H] - k_{-1}[C_6H_5CO_3^-][H^+] - k_2[C_6H_5CO_3H][C_6H_5CO_3^-] \approx 0$$

$$C_6H_5CO_3H \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C_6H_5CO_3^- + H^+$$

$$C_6H_5CO_3H + C_6H_5CO_3^- \xrightarrow{k_2} C_6H_5CO_2H + C_6H_5CO_2^- + O_2$$

$$C_6H_5CO_2^- + H^+ \xrightarrow{k_3} C_6H_5CO_2H$$

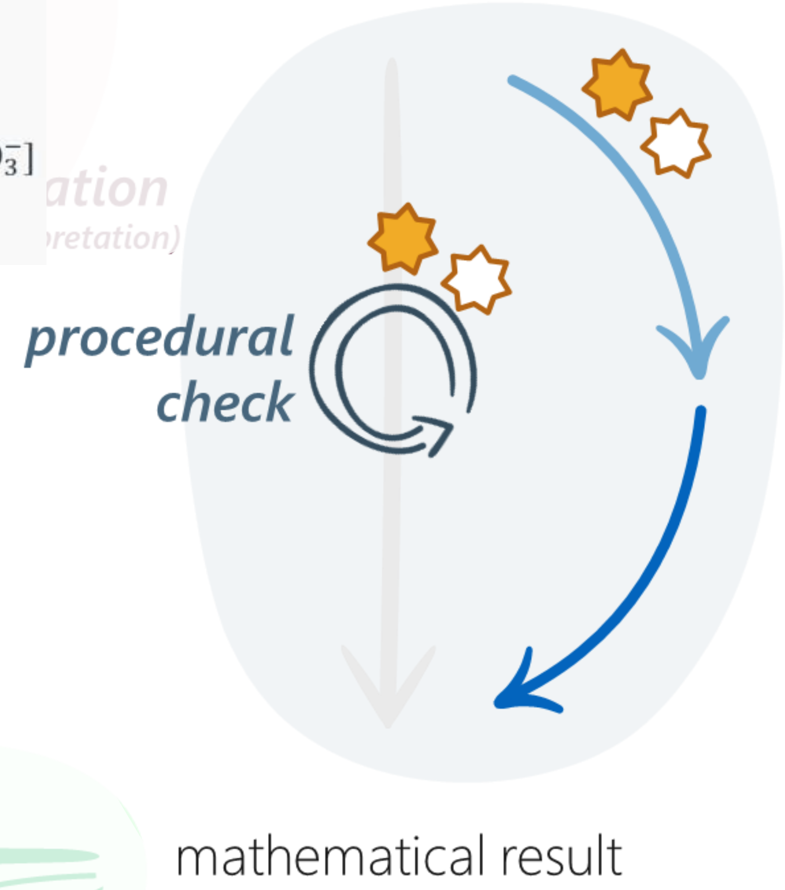


real model

mathematical model

$$\frac{d[O_2]}{dt} = k_2[C_6H_5CO_3H][C_6H_5CO_3^-]$$

$$\frac{d[C_6H_5CO_3^-]}{dt} = k_1[C_6H_5CO_3H] - k_{-1}[C_6H_5CO_3^-][H^+] - k_2[C_6H_5CO_3H][C_6H_5CO_3^-] \approx 0$$



MATHEMATICAL WORK

$$\frac{d[O_2]}{dt} = \frac{k_1 k_2 [C_6H_5CO_3H]^2}{k_{-1}[H^+] + k_2[C_6H_5CO_3H]}$$

validation

interpretation

validation
(no interpretation)

extra-mathematical resources (EMRs):

EVALUATION

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Deliberating, mathematics resources

E: Since we have a zero here… we can just set it up like… let's see now… [*silence*] This here is in both [$C_6H_5CO_3H$*, terms 1 and 3, expression 2*]… this here is in two [$C_6H_5CO_3^-$*, terms 2 and 3, expression 2*]… hm… What was it we do here then?

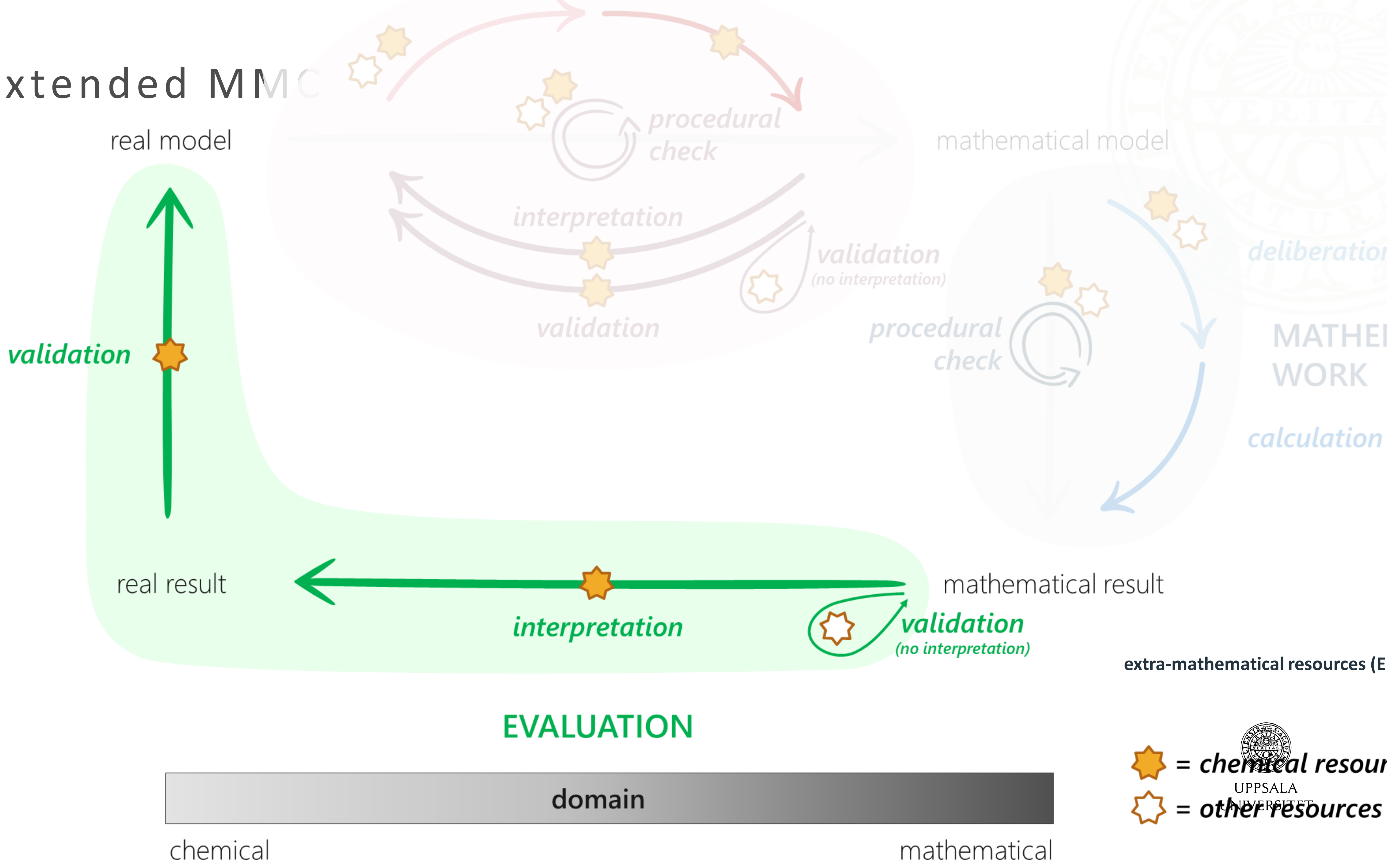
Deliberating, chemistry resources

E: OK, so the final goal is like… we want to be able to write this [$C_6H_5CO_3^-$*, term 2, expression 2*] in another way that only… is expressed in only that [$C_6H_5CO_3H$] and that [H^+]. Now, that [H^+] we don't want either since it's also an intermediate… only expressed in this [$C_6H_5CO_3H$], right?

Deliberating, other resources

E: … then we had something about that f**king symmetry that he talked about so that you can just like add them together or seomthing if you feel like it and everything is much easier.

The extended MMC



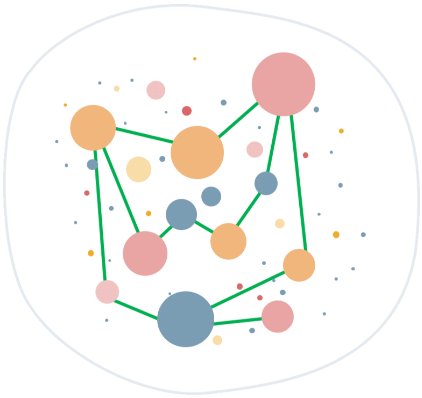
Interpretation and validation

$$\frac{d[\mathrm{O_2}]}{dt} = \frac{k_1 k_2 [\mathrm{C_6H_5CO_3H}]^2}{k_{-1}[\mathrm{H^+}] + k_2[\mathrm{C_6H_5CO_3H}]}$$

$$\mathrm{C_6H_5CO_3H} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{C_6H_5CO_3^-} + \mathrm{H^+}$$

$$\mathrm{C_6H_5CO_3H} + \mathrm{C_6H_5CO_3^-} \overset{k_2}{\rightarrow} \mathrm{C_6H_5CO_2H} + \mathrm{C_6H_5CO_2^-} + \mathrm{O_2}$$

$$\mathrm{C_6H_5CO_2^-} + \mathrm{H^+} \xrightarrow{k_3} \mathrm{C_6H_5CO_2H}$$



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Interpretation of physical meaning

G: Mm… and then we say that this [*oxygen production*] depends on… All of this [*rate law for oxygen production*] has a k_4 but it depends on… Let's see. It [*oxygen production*] depends on two different things – on how fast the concentration of the hydrogen and on the concentration of this [$C_6H_5CO_3H$] that I'm too tired to say.

H: Perbenzoic acid

G: Yes, squared.

Validation

Other resources

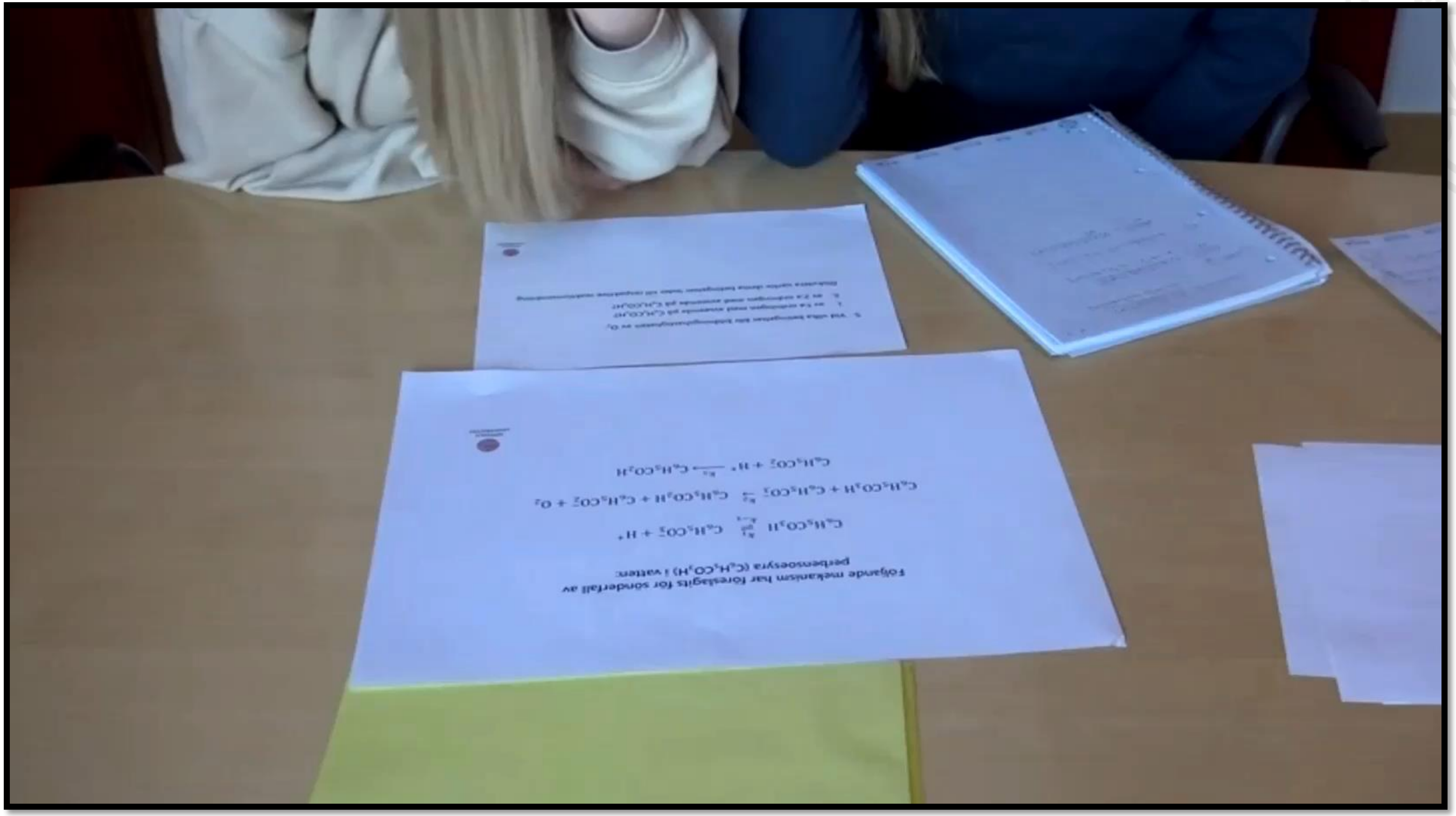
A: OK, erm… Or are we supposed to have such a long expression [*expression 6*]?

B: I don't know, it feels like that we could get something really… But then again, haven't we got such long expressions in like the tutorials?

A: Yeah, maybe we have? Sometimes you can just simplify it heaps… but I… but I don't know, I can't see at all how you could do that here…

Interpretation with validation

$$\frac{d[O_2]}{dt} = \frac{k_1 k_2 [C_6H_5CO_3H]^2}{k_{-1}[H^+] + k_2[C_6H_5CO_3H]} \approx k_1[C_6H_5CO_3H] \quad \text{if } k_2 \gg k_{-1}$$



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Some highlights of insights…

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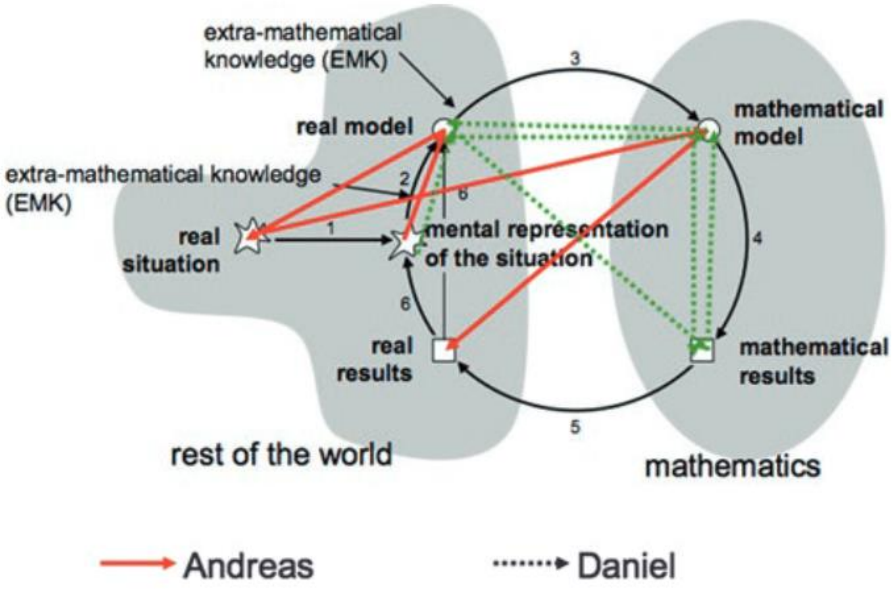
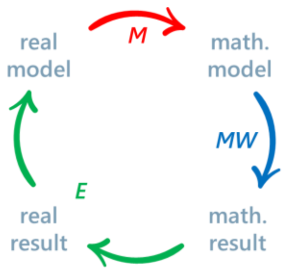
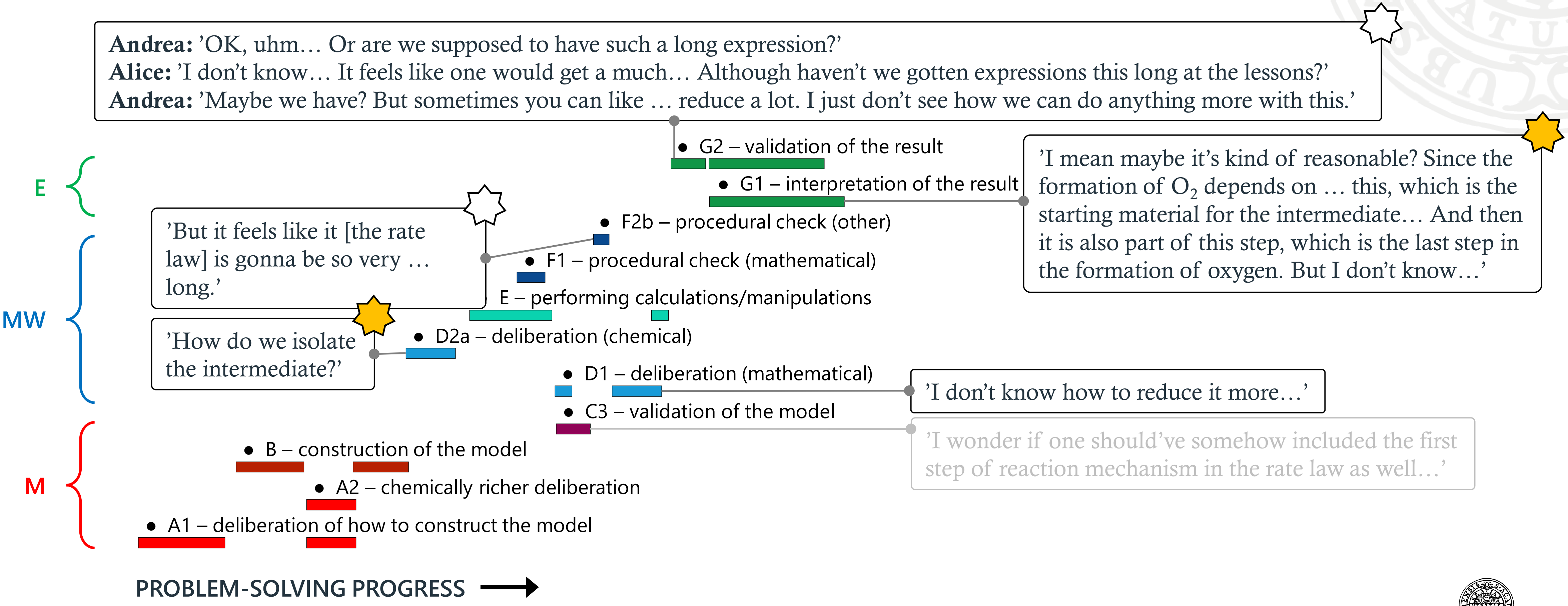
The model is idealised…



Doerr, Ärlebäck & Misfeldt, *International perspectives on the teaching and learning of mathematical modelling* **2017,** 71-81

Problem-solving trajectories





Alice & Andrea

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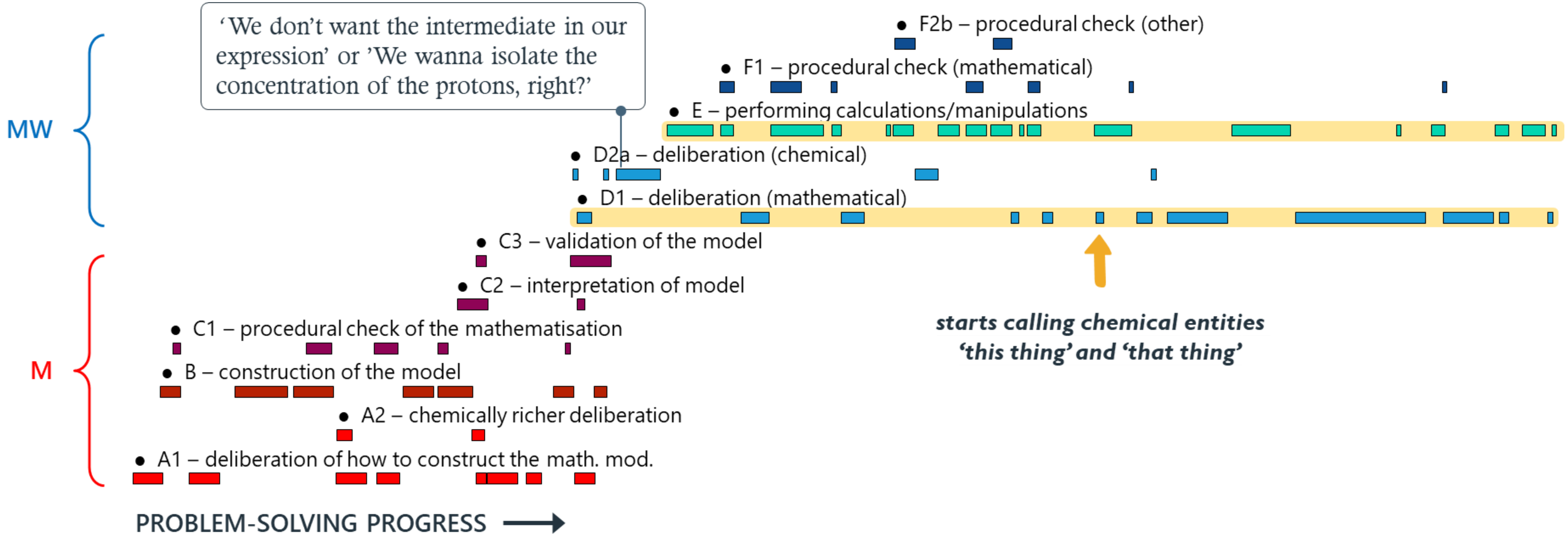
= chemical resources = other resources

Ye *et al*, *Chemistry Education Research and Practice* (2024), **25**, 242 - 265

Being *'good at maths'* is not enough!



David & Diana

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Ye *et al*, *Chemistry Education Research and Practice* (2024), **25**, 242 - 265

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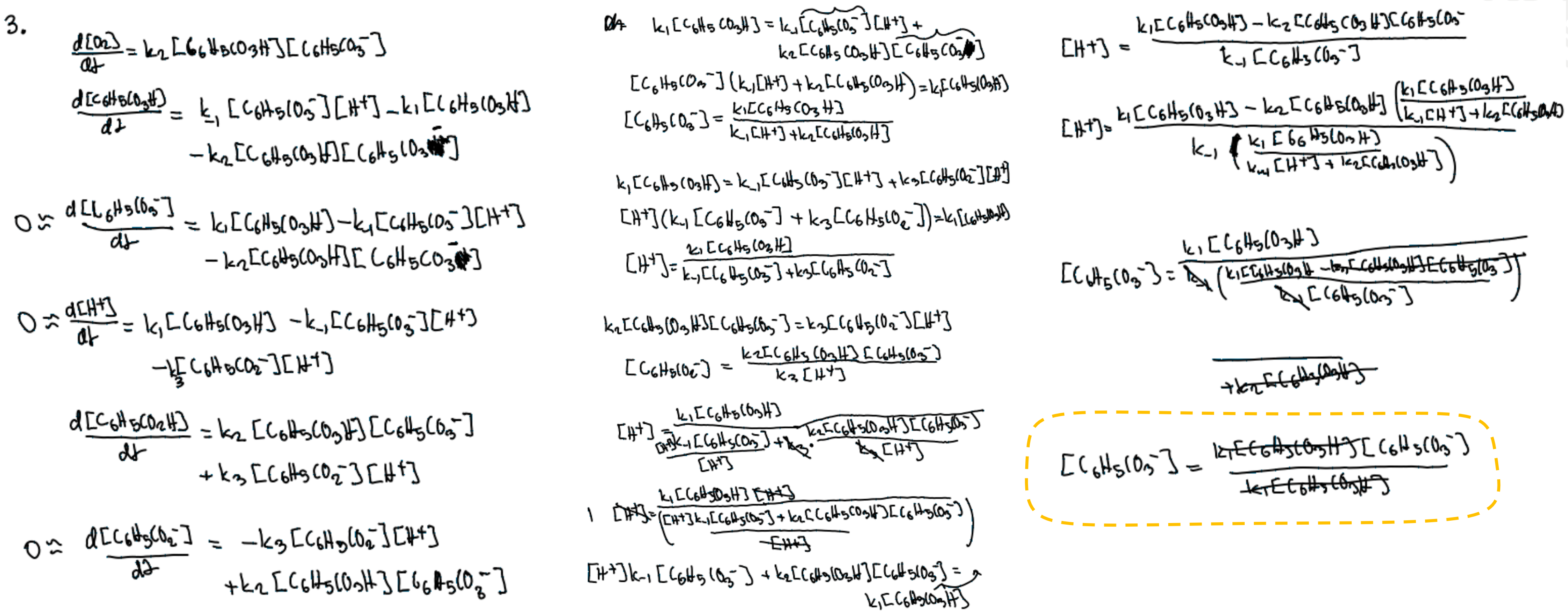

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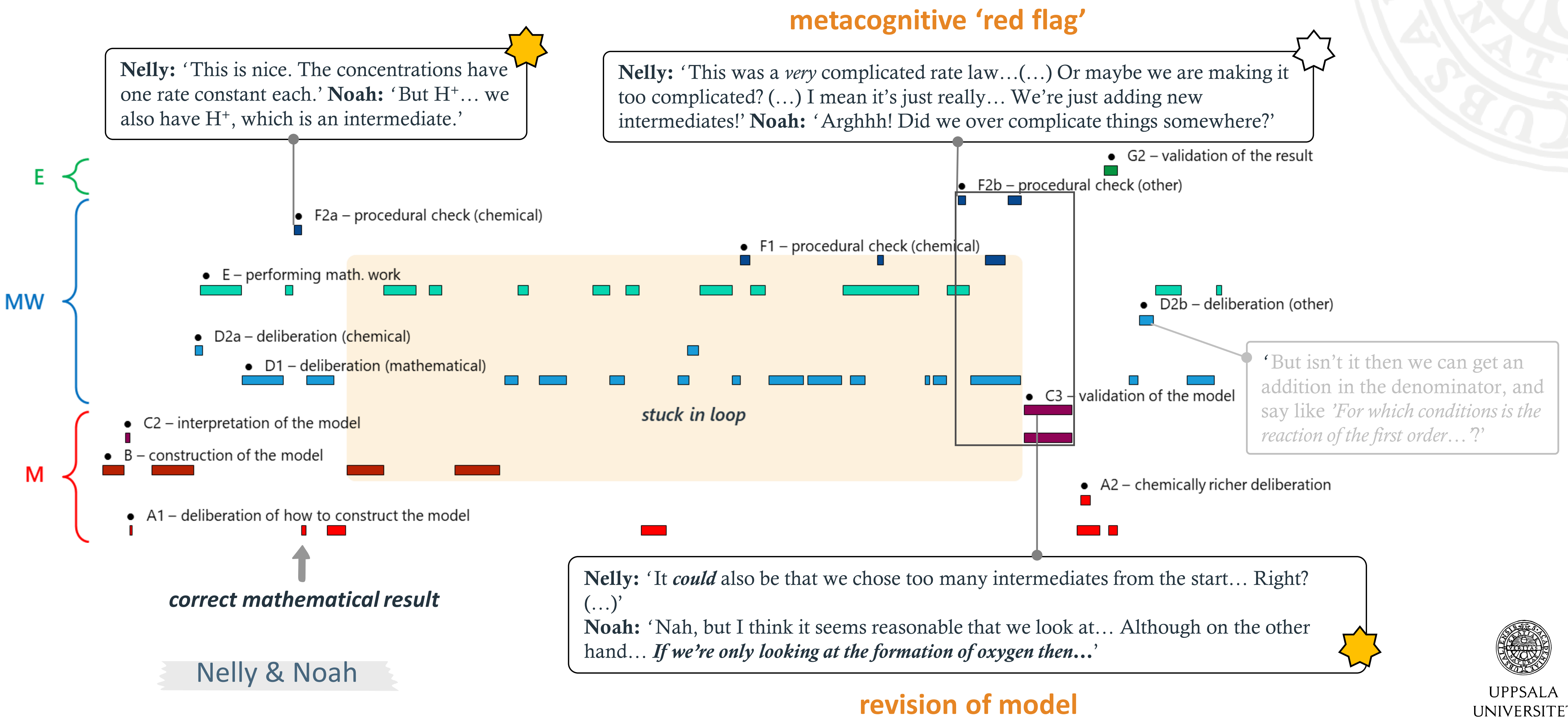
Ye *et al*, *Chemistry Education Research and Practice* (2024), **25**, 242 - 265

EMRs can help students *'Get back on track'*!



= chemical resources = other resources

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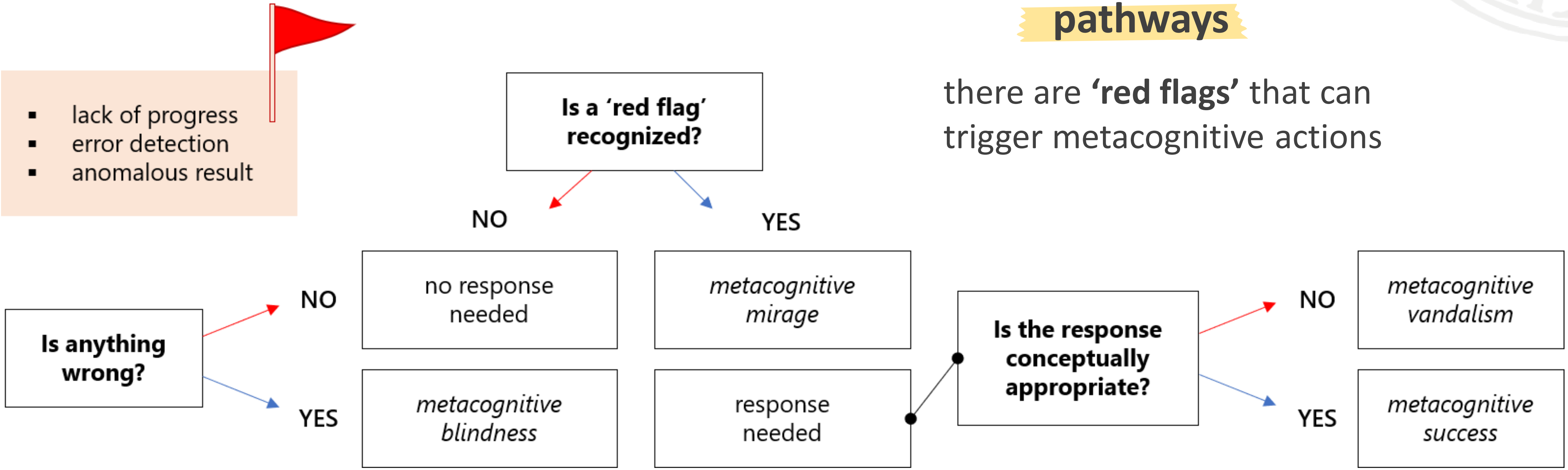
Ye *et al*, *Chemistry Education Research and Practice* (2024), **25**, 242 - 265

Moments of uncertainty,
metacognitive red-flags and intuition

metacognitive pathways

there are **‘red flags’** that can trigger metacognitive actions



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Goos, *The Journal of Mathematical Behaviour* **2002,** *21*, 283-302

There's more than explicit or strict content knowledge

implicit models of results

'This was a *very* complicated rate law, or are we *making* it too complicated?'

'But it feels like it's going to be really very long...?'

explicit examples from experience/episodic memory

'… then we had something about that f**king symmetry that he talked about …'

'But then again, haven't we got such long expressions in like the tutorials?'

- Helped students identify possible issues, or provide reassurance
- Compare with expert behaviour and intuition

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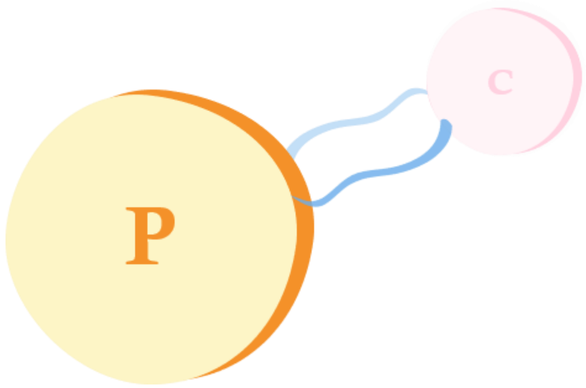
Ye *et al, manuscript in preparation*

Relationship between procedural and conceptual resources

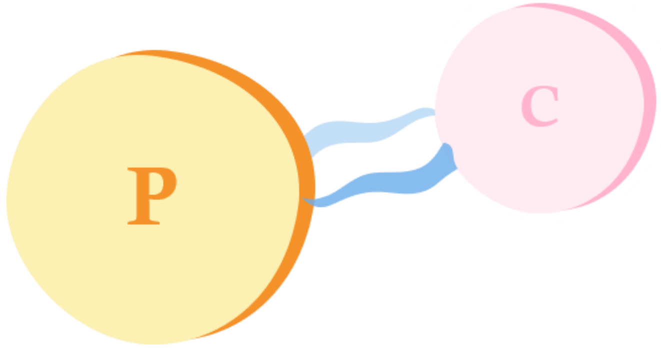
WEAK

They know how, but give no indication why it is appropriate.



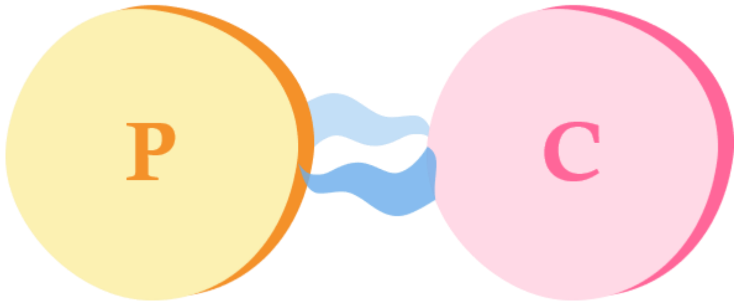
MODERATE

They know how, and give some indication why it is appropriate.



STRONG

They know how, and justify conceptually why it is appropriate.



”Plug ’n chug”

Ye *et al, manuscript in preparation*

From an on-going study focusing on mathematisation…

You are studying a reaction with the net equation: $\boldsymbol{X} \rightarrow \boldsymbol{P}$. Using the given absorbance data, determine the reaction order of the consumption of X.

Table 1. Absorption coefficients.

λ (nm)	300	350	375	450
ε_P / L mol^{-1} cm^{-1}	0,00	1,27	3,27	11,1

λ (nm)	300	350	375	450
ε_X / L mol^{-1} cm^{-1}	16,8	6,38	3,87	0,00

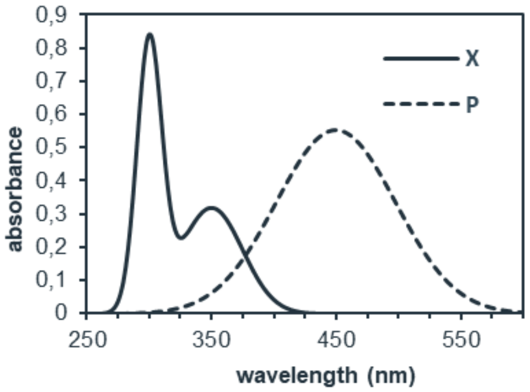
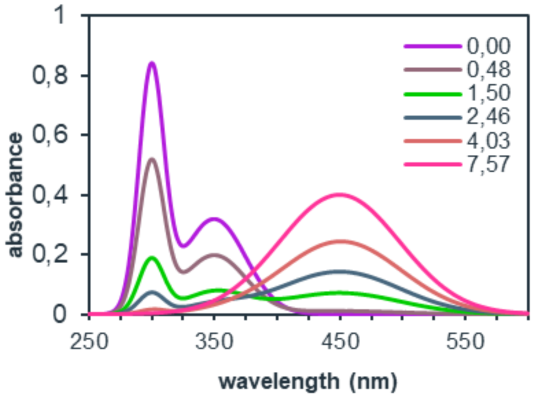


Table 2. Abs at λ = 375 nm and λ = 450 nm. Only X is present at t = 0.

t (min)	Abs (375 nm)	Abs (450 nm)
0,00	0,194	0,000
0,48	0,123	0,011
1,50	0,064	0,072
2,46	0,059	0,142
4,03	0,076	0,247
7,57	0,119	0,402



What is the concentration of X at different points in time?

$$A = \varepsilon c l$$

$$A(t)_{300} = \varepsilon_{X_{300}} \boldsymbol{c_X(t)} l$$

$$A(t)_{375} = A_X + A_P$$

$$= \varepsilon_{X_{375}} \boldsymbol{c_X(t)} l + \varepsilon_{P_{375}} c_P(t) l$$

$$\boldsymbol{c_X(t)} = \frac{A(t)_{375} - \varepsilon_{P_{375}} c_P(t) l}{\varepsilon_{X_{375}} l}$$

Chemical concepts = absorbance (familiar)

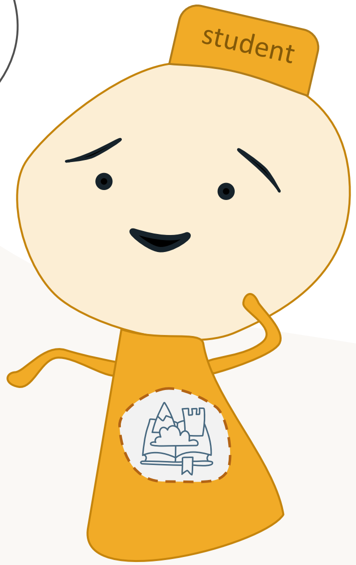
Mathematical work = basic arithmetic operations (familiar)

Mathematisation = translation of time-dependent chemical phenomena to an appropriate mathematical model (unfamiliar)

Just because you can, doesn't mean you should…

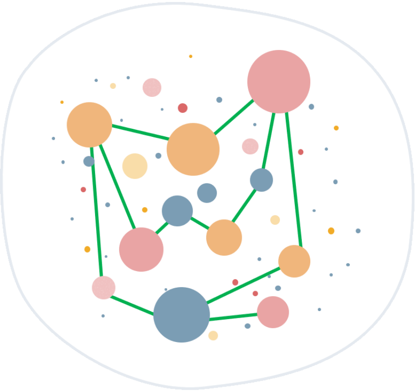
We see influences from students' **epistemological resources**, for example:

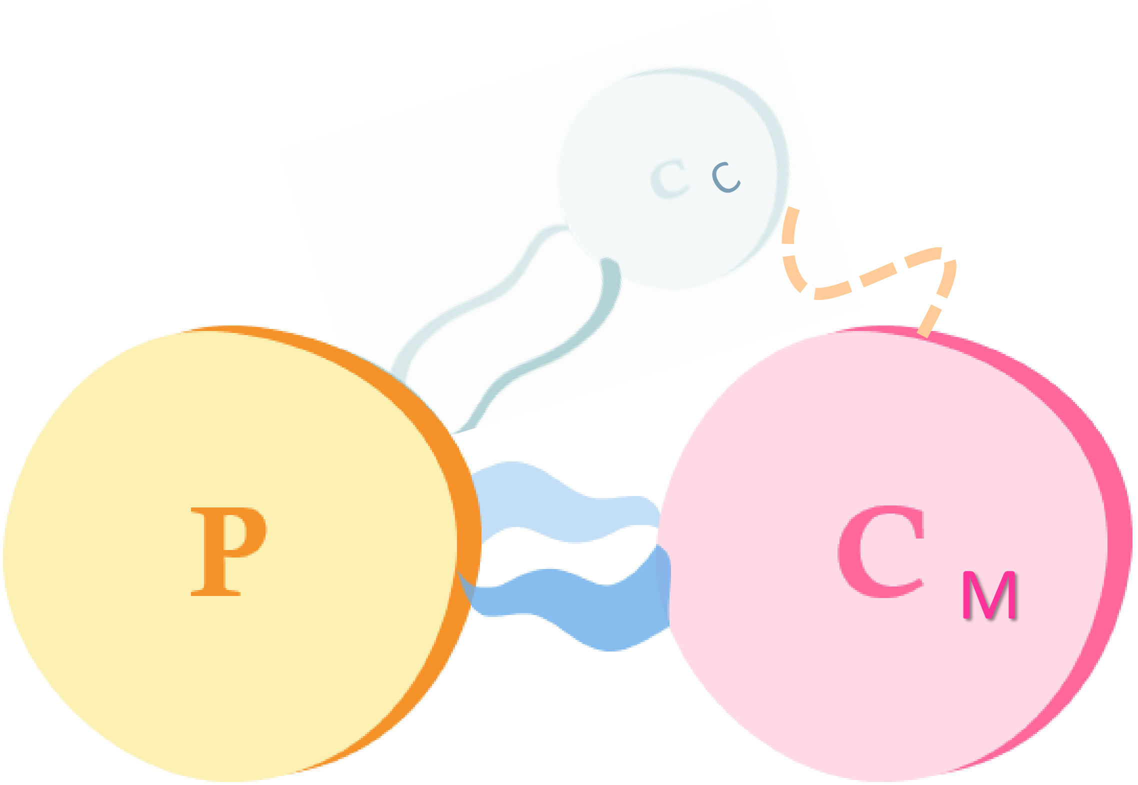
"I was thinking we could try that… But I thought it was ***illegal!****"*



"The maths wasn't difficult to grasp but it's difficult to do it when you hadn't seen it before!"

Determining which parameters to mathematise is at least as challenging as the mathematisation itself.





What is it that's going on here?

Ye et al, manuscript in preparation

University teachers' conception of the role of mathematics in non-mathematical disciplines - a phenomenographic study

- Tension between teachers' and students' views
- Tension between the reasons and goals for what, why and how mathematics is taught

A philosophical foundation

An agent for development

A key to understanding

A language for communication

A computational tool

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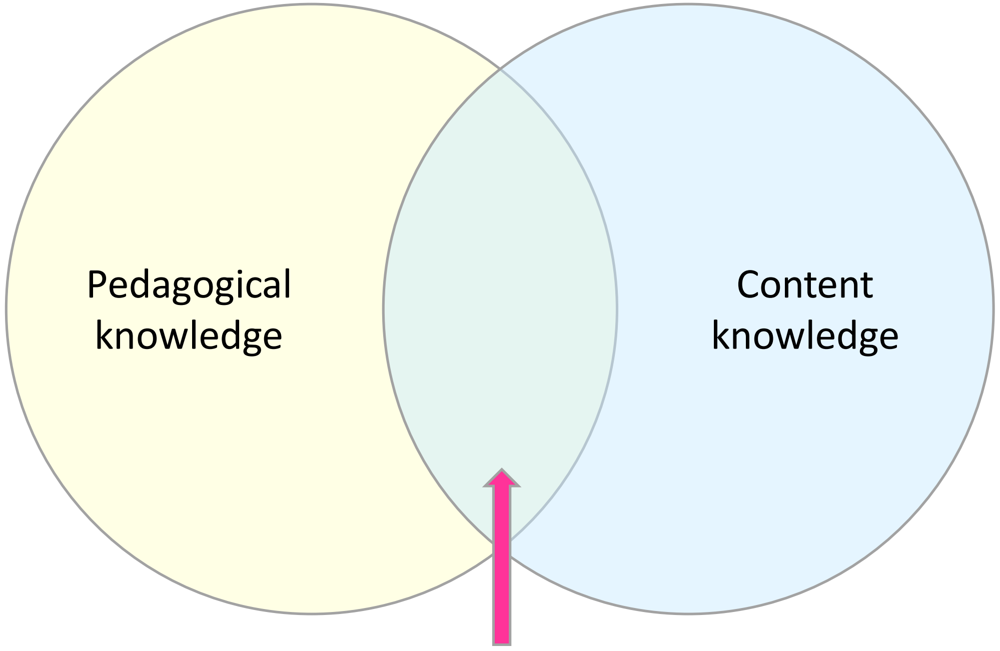
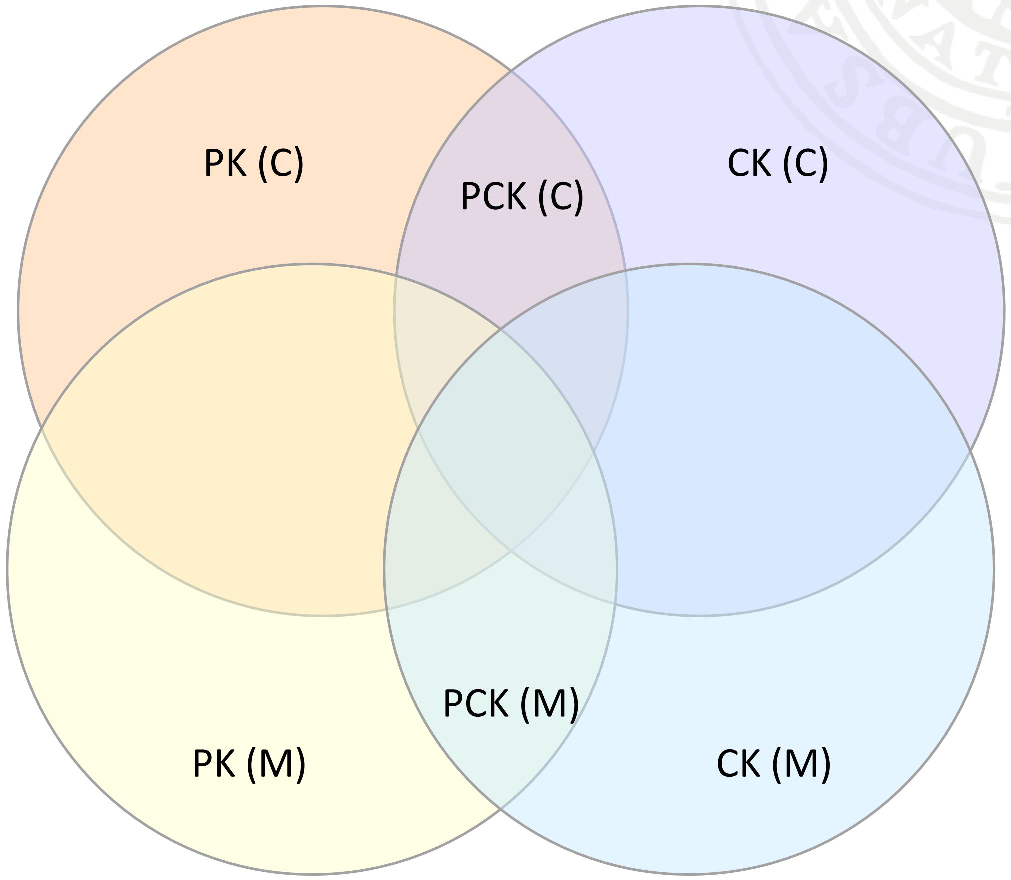
Koeffer, Polverini et al (2024, soon submitted)

Who should teach "the intersection"? What should be taught?





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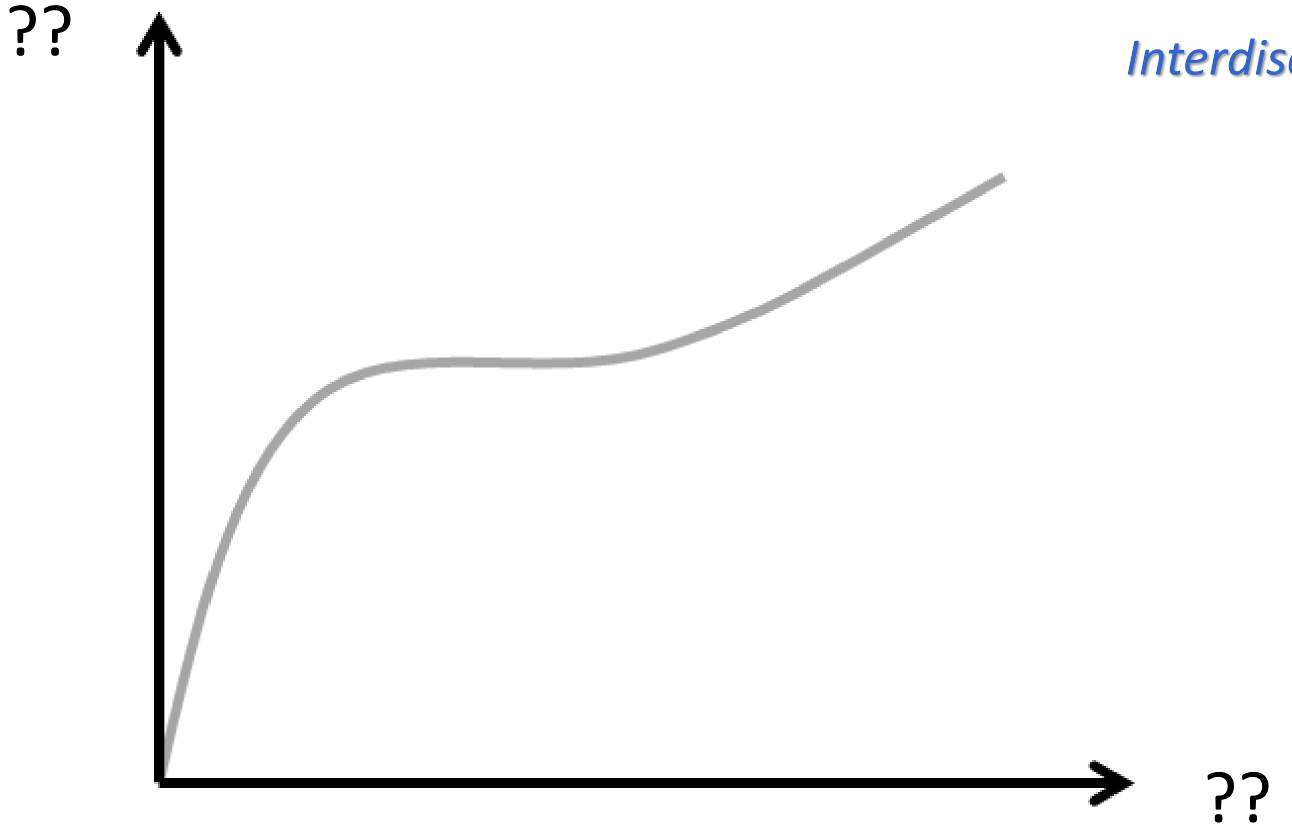
Shulman (1986), Kind & Chan (2019)

Who should teach ”the intersection”?
What should be taught?

What questions can be asked?

Why teach what, how, by whom?

Interdisciplinary collaborations



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~~The "anti-cliffhanger"~~ *(Attempted) Summary*

- It's much more than teaching and learning the "right" maths and the "right" chemistry
    - A range of subprocesses during the problem-solving process with intricate involvement of various disciplinary and non-disciplinary resources
    - Appropriate activation, productive application and different roles of resources in problem solving
    - "Being good at" or productive applicaton of maths interact highly with the disciplinary context
    - Deciphering physical significance in mathematical formalisms, judgement in context
    - Importance of metacognitive control, development of expertise and intuition
- There are numerous issues concerning aims and goals for teaching and learning that effect the answer to how mathematics education in/for other disciplines should be approached
    - How do teachers themselves conceive the role of maths, how is this communicated
    - Important questions of what, why, how and by whom

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