Introductory Chemical Dynamics—Using the Chemical Potential from the Start

An Informal Introduction to Chemical Processes

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THE GOAL OF THIS TALK…

Taditionally, it is assumed that the chemical potential can only be introduced—and understood—as a derived quantity.

In this talk, I would like to motivate the view that the chemical potential is one of the quantities we should take as **primitive**, meaning, as fundamental, basic, *not derivable and not derived* from other (seemingly) more fundamental concepts.

Any discussion of such a point—why should we introduce a particular quantity as primitive, and how can we do this?—has emotional quality. Therefore, I will use a good part of my presentation to motivate the concept of chemical potential by discussing basic human conceptualizations of nature. These conceptualizations have been identified in recent research in cognitive science in general, and cognitive linguistics in general. They will then be applied to chemical processes leading to the identification of the chemical potential as a measure of the intensity of chemical processes.

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Contents

Part 1

INTRODUCTION: CHEMICAL PROCESSES

Chemical processes are those that deal with the **quantity** of substances, their strength or **intensity** relative to each other, and their **power** to cause other phenomena…

WORD MODELS OF CHEMICAL PHENOMENA

EXAMPLE	A WORD MODEL
Osmosis in potatos	Should you cook potatoes in **lightly** saltet water or in **strongly** salted water? It turns out that in fresh water, potatoes swell, in strongly salted water they shrink. Water **flows** into or out of the potatos: it **forced** from places where it is purer to be where there is more stuff dissolved in it. So what is the best way to cook potatoes? Shouldn't we try to avoid a major exhange of water by using just the **right amount** of salt? If we want to leave the roots in their original state, we should try to go for a sort of **balance** between the inside of the potatoes and their environment.
Melting of ice	The substance H2O **transforms** from liquid to solid if the temperature of the environment is below 0°C, and it has a **tendency** to go from solid to liquid if it is warm. It seems, H2O "**likes**" to be in the liquid state when it is warm, and it "prefers" to be in the solid state when it is cold. There is a point of **balance** between liquid and solid at 0°C.

EXAMPLE	A WORD MODEL
Detergents and washing clothes	Want to clean dirty clothes? Depending on the type of stains, you might need some **aggressive** soap, in other cases, a **mild** degergent should be enough. Some soaps are more **powerful** than others. Clearly, if you have more clothes to wash, you need **more** detergent.
Batteries	In batteries, chemicals are brought in contact in such a way that electricity flows when they react. The **intensity** of the reaction—which depends upon the particular chemicals—determines the electric potential difference, i.e., the electric "**tension**." **More** of the same chemicals allow the battery to live longer, i.e., to pump more charge. The **kind** and the **quantity** of chemicals determine the **power** of a battery.
Burning fuels	Fuels produce heat when burned. If we want more heat, we need **more** fuel, or a better ("**stronger**") fuel. The **power** of heating depends upon the type of fuel and how fast the fuel is burned.

Part 2

Conceptualization of Processes—Force Dynamic Gestalts

Human perception leads to the abstraction of a structured gestalt of experiences as diverse as love, pain, heat, or motion. The aspects of the gestalt are **quantity**, **intensity**, and **power/force**. I call them *Force Dynamic Gestalts*.

Quantity, intensity, and power (and associated schemas such as driving force, flow, container, resistance, balance…) are the basic concepts of a continuum physics approach to natural phenomena.

THE FORCE DYNAMIC GESTALT OF ABSTRACT CONCEPTS

Concepts such as **evil** or **love** or **thought** are abstracted from experience in the form of a preconceptual structured **Force Dynamic Gestalt** having the aspects of

Substance (quantity) / Intensity (quality) / Force or Power

Linguistic expressions for evil:

- She had no idea how strong evil could be.
- Evil burned intensely.
- Evil grew amongst us.
- Evil gained control of this group of people.
- Slowly, evil left his soul.
- Evil made him do things he would not have done otherwise.

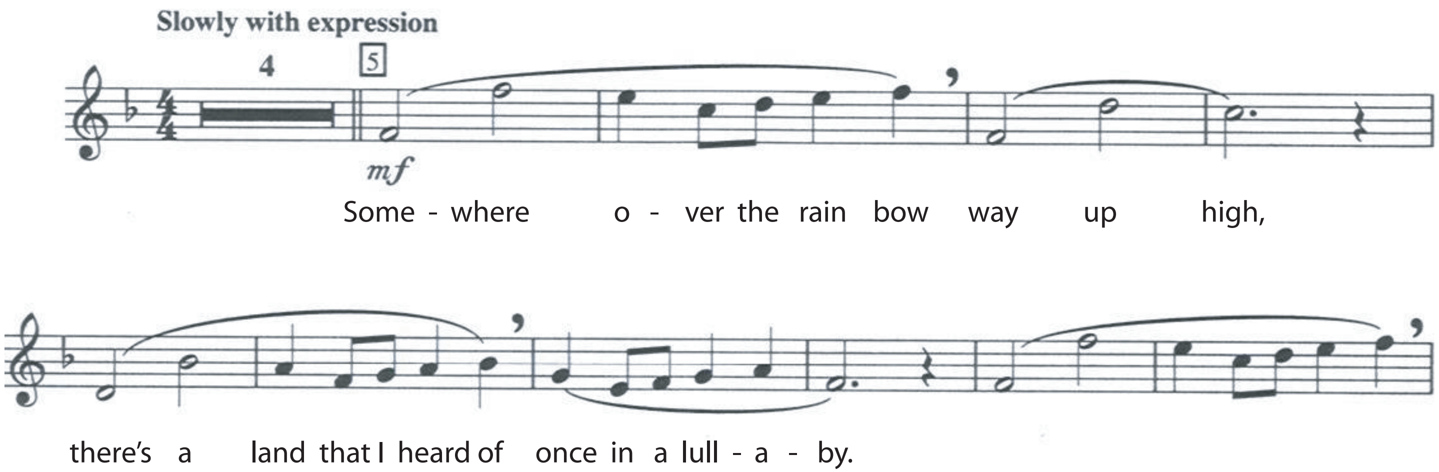
Entailments of the conceptualization

Two bad people means double the evil. More evil means higher intensity. More evil means it is more powerful. Higher intensity of evil increases its power.

THE METAPHORIC CONCEPTUALIZATION OF MUSIC

Music is conceptualized by three main metaphoric projections of schemas (Mark Johnson: *The Meaning of the Body. Aesthetics of Human Understanding*. The University of Chicago Press, Chicago, 2007):

- The moving music metaphor (“Here comes the recapitulation.”). **Object**
- The musical landscape metaphor (“The melody rises up ahead.”). **intensity**
- Music as moving force metaphor (“This piece moved me to tears”). **Force or power**



EVIDENCE FOR THE GESTALT OF PHYSICAL PROCESSES 1

Persons are asked if they agree or disagree with certain expressions

- The temperature is high
- Today, the heat is high
- There is lots of heat in this room
- There is lots of temperature in this room
- Heat drives the engine
- Temperature drives the engine

Agreement with classes of expressions[a]

	as substance	as level	as cause
Heat	**0.67 (1)**	**0.14 (0)**	**0.77 (1)**
Temperature	**0.09 (0)**	**0.83 (1)**	**0.09 (0)**

a. Agreement (1) or disagreement (0) with expressions using heat and temperature. Expected results in parentheses. Results of a questionnaire given to journalism students in Summer of 2004.

EVIDENCE FOR THE GESTALT OF PHYSICAL PROCESSES 2

The concept of heat in the Accademia del Cimento

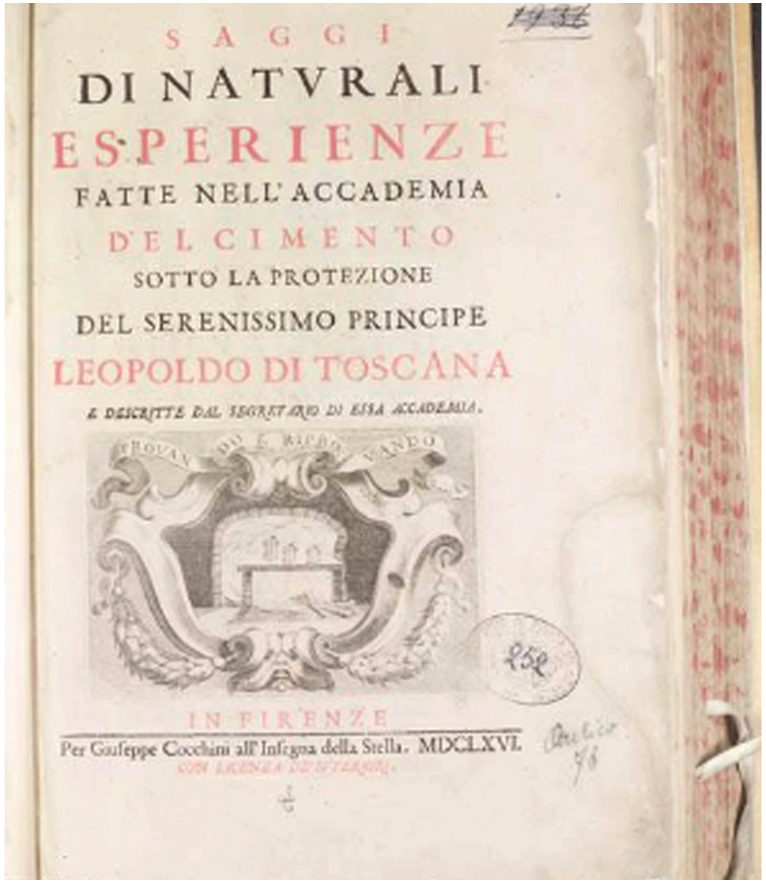
The concept of heat of the members of the Accademia del Cimento: Saggi di naturali esperienze… (1667)

M. Wiser and S. Carey (1983): When Heat and Temperature were one.

“The Experimenters’ concept of heat had three aspects: **substance** (particles), **quality** (hotness), and **force**.”

A weakly differentiated gestalt

It seems that the Experimenters did not really distinguish between these aspects of the gestalt of heat.



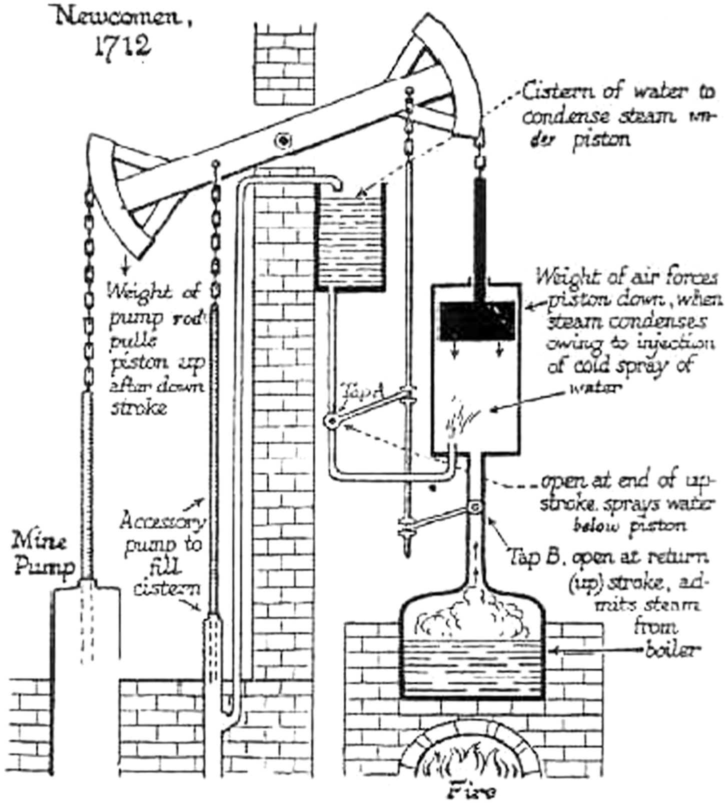
EVIDENCE FOR THE GESTALT OF PHYSICAL PROCESSES 3

Sadi Carnot's Image of the Power of Heat

Sadi Carnot (1796-1832)
Réflexions sur la puissance motrice du feu

An example of a fully differentiated Force Dynamic Gestalt

D'après les notions établies jusqu'à présent, on peut comparer avec assez de justesse la *puissance motrice de la chaleur* à celle d'une chute d'eau […]. La puissance motrice d'une chute d'eau dépend de sa hauteur et de la quantité du liquide; la puissance motrice de la chaleur dépend aussi de la quantité de calorique employé, et de ce qu'on pourrait nommer, de ce que nous appellerons en effet *la hauteur de sa chute*, c'est-à-dire de *la différence de température* des corps entre lesquels se fait l'échange du calorique.



DIAGRAMMATIC VIEW OF NEWCOMEN'S ATMOSPHERIC OR FIRE ENGINE (1712)

THE FORCE DYNAMIC GESTALT OF PHYSICAL PROCESSES

Human perception of phenomena such as fluids, electricity, heat, motion

The concept of “heat,” for example, is abstracted by perception from the sum total of thermal experiences in the form of a **gestalt**: An entity that is simpler than the sum of its parts. While we do not differentiate a gestalt of a collective of phenomena (such as electricity or heat) consciously, we do notice aspects. The most fundamental **aspects** humans use to talk about such a **gestalt** are

Table 1: The Force Dynamic Gestalt of collectives of physical phenomena

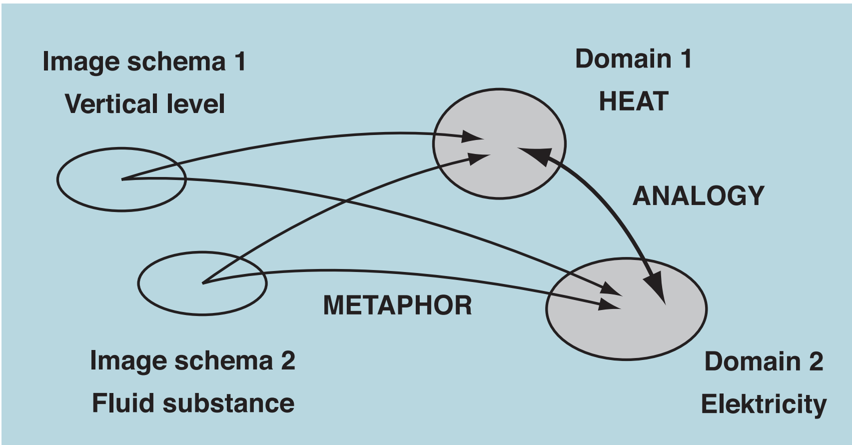
ASPECT OF GESTALT	METAPHORIC STRUCTURE
Intensity (quality)	Polarity such as light-dark, warm-cold, high-low, fast-slow, strong-weak. The concepts are structured metaphorically by the **image schema** of verticality (intensity as a level).
Quantity (substance)	Substance-like (or fluid-like) concepts are metaphorically structured in terms of the **image schema** of fluid substances.
Force or power	Prototypical **causation** as the gestalt of direct manipulation.

Metaphors and analogical reasoning

Origin and meaning of analogies

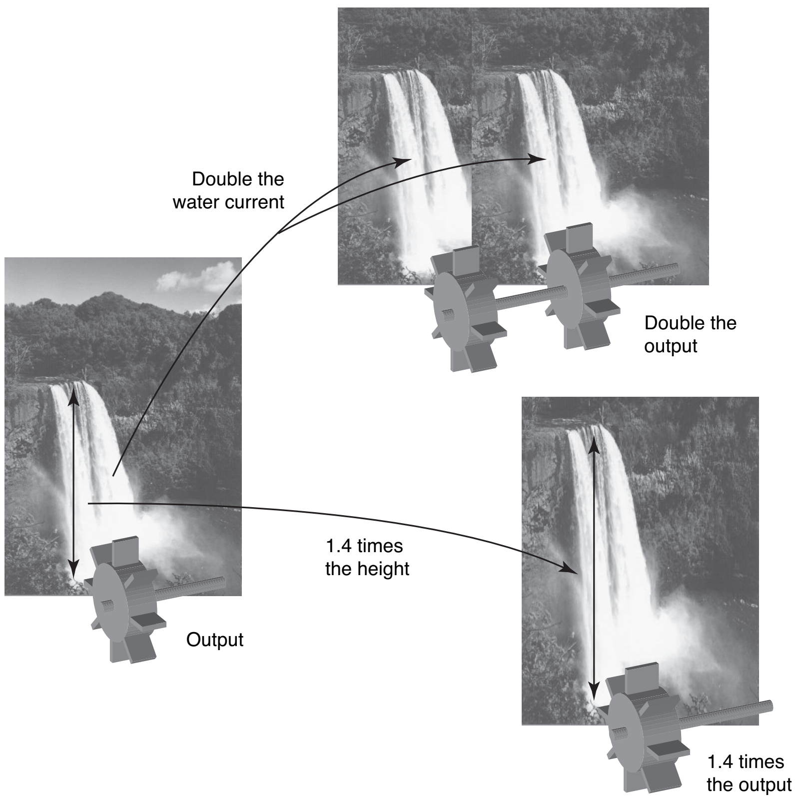
When different domains of experience are structured metaphorically by the same source domains (such as by the same image schemas), these domains become comparable (they are looking similar).

This comparison can be applied in the construction of analogies. An analogy is a double-sided mapping (more or less symmetrical).



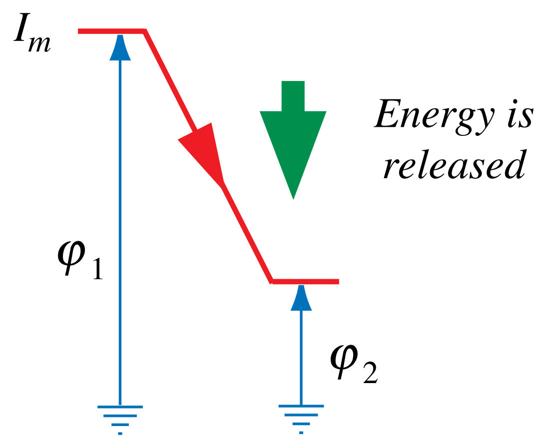
ENTAILMENTS OF THE FORCE DYNAMIC GESTALT OF PHYSICAL CONCEPTS

An example of entailments that can be brought into quantitative form



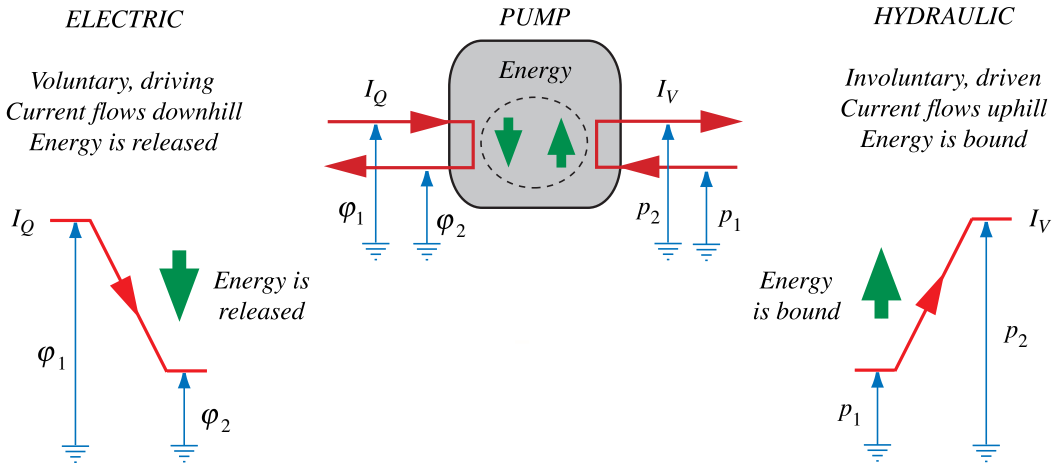
$$Power =$$

$$Level\ difference \cdot Current\ of\ substance$$

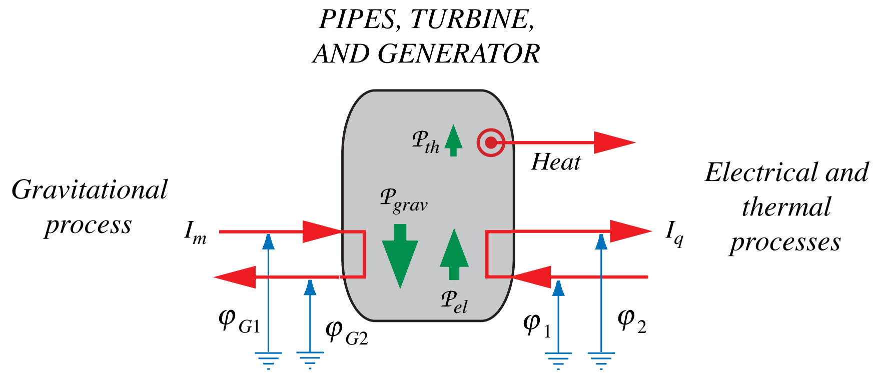


The Waterfall Image in Process Diagrams

- **Ideal coupling**

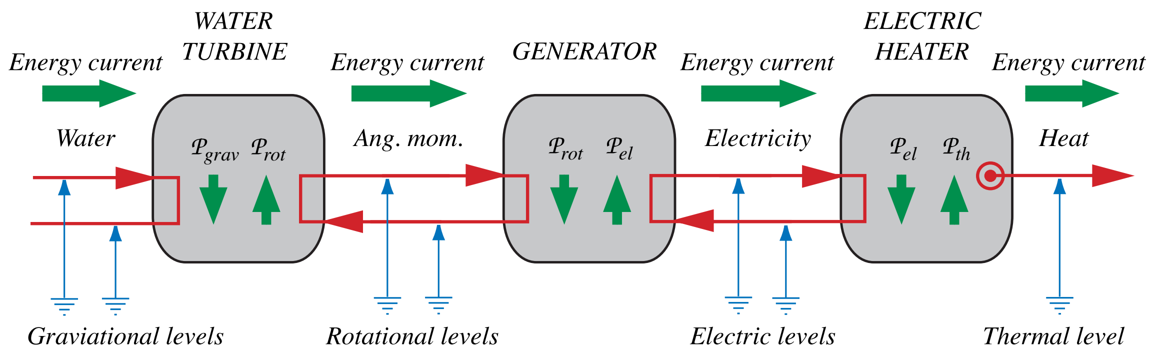


- **Real coupling**

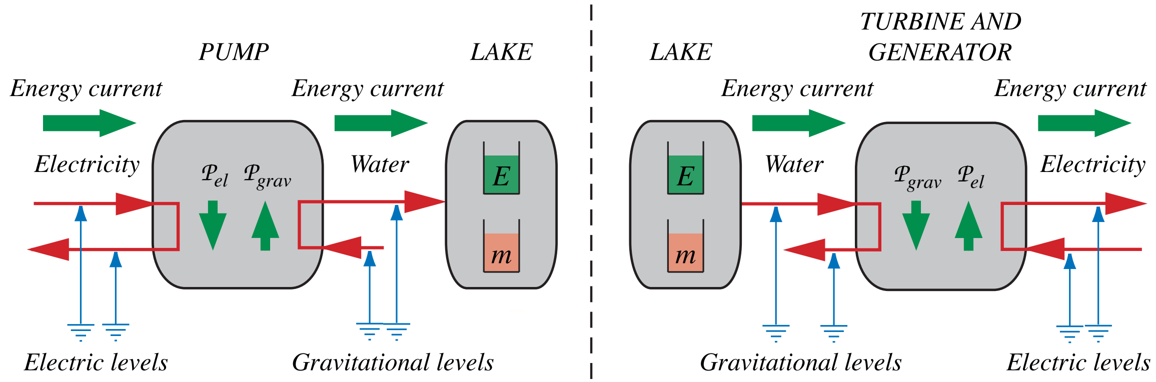


Energy Flow and Storage in Process Diagrams

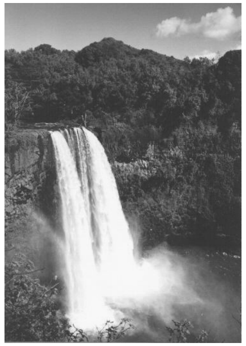
- **Transport of energy**

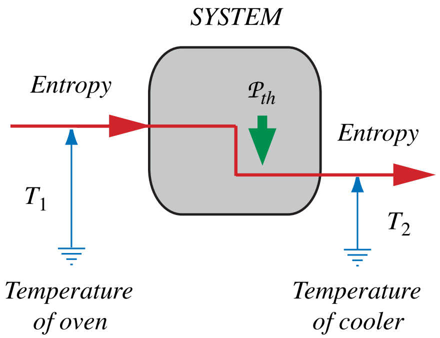


- **Energy storage**

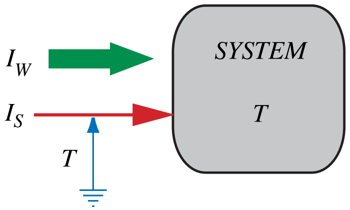


ENERGY IN THERMAL PROCESSES

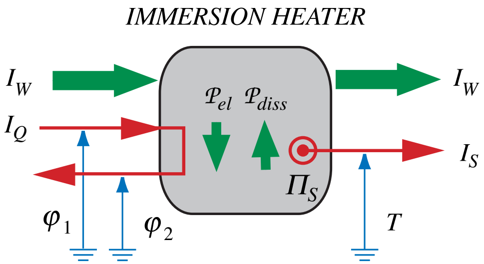




Thermal power= Temperature difference· Entropy current



Energy current in heating and cooling= Temperature · Entropy current



Dissipation rate= Temperature · Entropy production rate

Part 3

CONCEPTUALIZING CHEMICAL PROCESSES

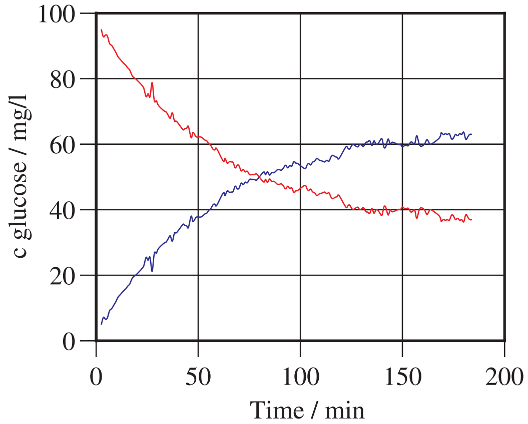
Chemical processes are those that deal with the quantity of substances, their strength or intensity relative to each other, and their power to cause other phenomena…

It appears quite reasonable to assume that chemical processes are conceptualized with the help of the same Force Dynamic Gestalt that proved its utility in other prcesses…

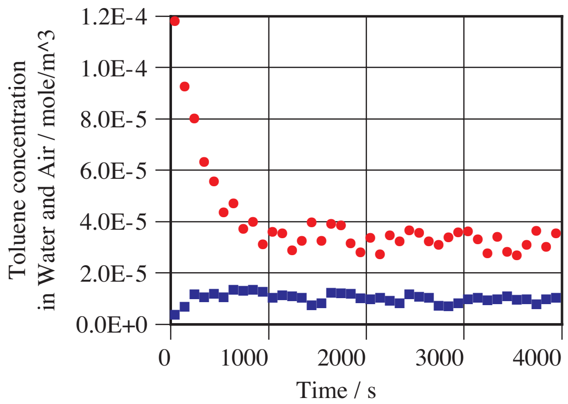
Motivating the Concept of Chemical Potential and Chemical Driving Force

	Observation and explanation
Air and Water	When dry air flows over warm water, the air picks up water (vapor). There is a **driving force** for the transfer of water into the (dry) air.
Water and Ice	At a temperature of 25°C, water does not turn to ice, ice turns to water: H2O “**likes** better” to be in the liquid state. At a temperature of 0°C, there is neither a tendency for water to turn into ice nor a tendency for ice to turn into water: we have a state of **equilibrium**.
Producing Metal Sulfides	When Mg (magnesium), Zn (zinc), iron (Fe), and copper (Cu) are made to react with sulfur (S), metal sulfides are produced. The intensity of the reactions is very different, with Mg the most violent, and Cu the least active. Clearly, we need a measure of **intensity** (or difference of intensities) to explain this result.
Burning Fuels	For the same amount of fuel burned, vastly different amounts of heat can be produced: we need a measure of **intensity** of the reaction.
α-Glucose and β-Glucose	If there is only α-glucose in an aqueous solution, it turns into β-glucose: there is a **driving force** of the reaction. The **stronger the driving force**, the **faster** the reaction. If the anomers are in a particular proportion (roughly 40:60), there is no conversion: we have **equilibrium**.

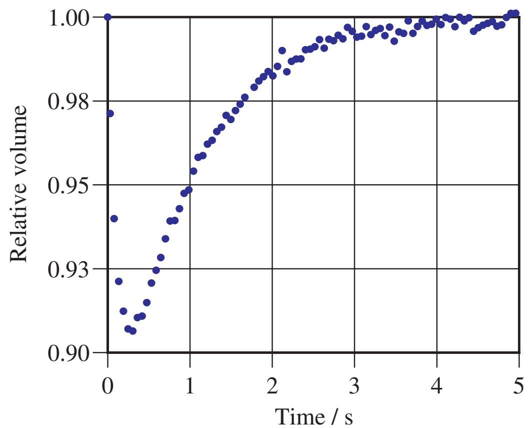
Motivating the Concept of Chemical Potential and Chemical Driving Force



Mutarotation
of glucose



Toluene in
water and air

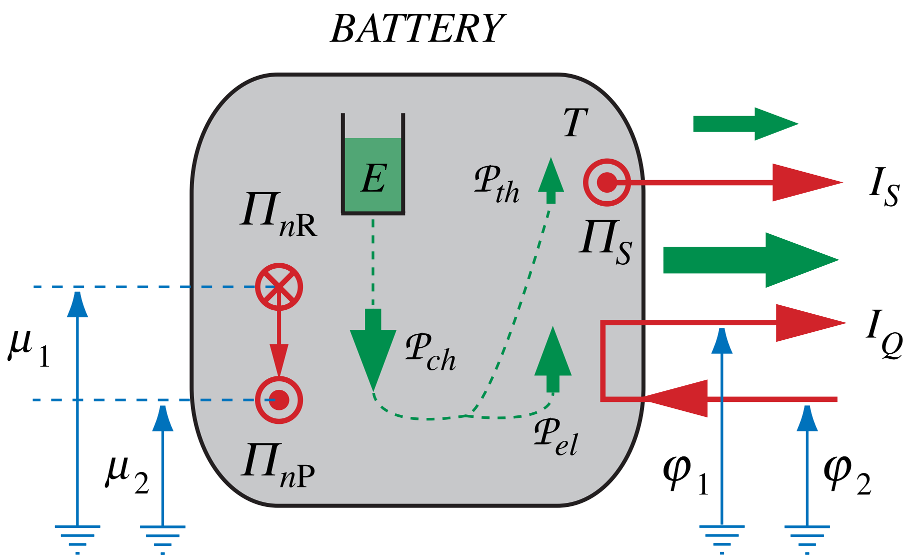


Volume of red blood cells
in an aqueous solution

ANALOGIES: SUBSTANCE-LIKE QUANTITIES, POTENTIALS, AND POWER

	Substance-like quantity	**Current of quantity Production rate**	**Associated power**
HYDRAULICS	Volume of liquid	Volume current	$\mathcal{P} = \Delta p I_V$
ELECTRICITY	Electric charge	Current of charge	$\mathcal{P} = \Delta \varphi_{el} I_Q$
THERMODYNAMICS	Entropy	Entropy current Entropy production rate	$\mathcal{P} = \Delta T I_S$ $\mathcal{P}_{diss} = T \Pi_S$
ROTATION	Angular momentum	Angular momentum current	$\mathcal{P} = \Delta \omega I_V$
TRANSLATION	Momentum	Momentum current	$\mathcal{P} = \Delta v I_V$
GRAVITATION	(gravitational) mass	Current of mass	$\mathcal{P} = \Delta \varphi_g I_m$
CHEMISTRY	Amount of substance	Current of amount of substance Production rate of n	$\mathcal{P} = \Delta \mu I_n$ $\mathcal{P} = \Delta \mu \Pi_n$

PROCESS DIAGRAMS: A SYSTEM INVOLVING CHEMICAL REACTIONS



Process diagram of a battery, including production of entropy.

There is no energy transfer relative to the system with chemical substances.

Energy released in the reactions comes from energy storage.

The power of the chemical process is split between the electrical and thermal processes.

$$\mathcal{P}_{chem} = [\Delta\mu]_R \, \Pi_n$$

THE CHEMICAL DRIVING FORCE

REACTION:

$$\nu_1 \mathrm{A}_1 + \nu_2 \mathrm{A}_2 + \ldots \leftrightarrow \varsigma_1 \mathrm{B}_1 + \varsigma_2 \mathrm{B}_2 + \ldots$$

DRIVING FORCE:

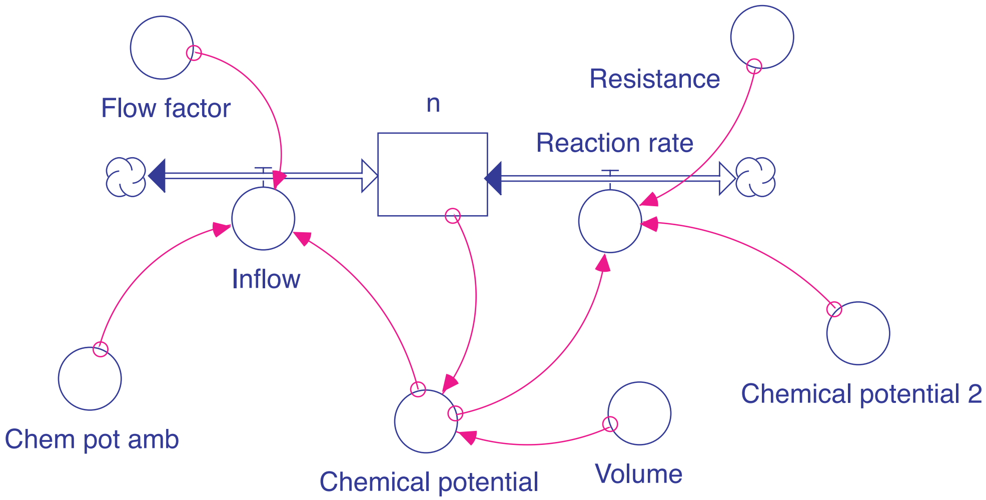
$$\left[\Delta\mu\right]_R = \varsigma_1 \mu_{\mathrm{B1}} + \varsigma_2 \mu_{\mathrm{B2}} + \ldots - \left(\nu_1 \mu_{\mathrm{A1}} + \nu_2 \mu_{\mathrm{A2}} + \ldots\right)$$

Voluntary process $\left[\Delta\mu\right]_R < 0$

Involuntary process $\left[\Delta\mu\right]_R > 0$

Chemical equilibrium $\left[\Delta\mu\right]_R = 0$

Conceptualizing Dynamical Chemical Processes



$$\Pi_n = \frac{1}{R_n}\left[\Delta\mu\right]_R$$

$$I_n = G_n\left[\Delta\mu\right]_R$$

System dynamics model diagram of chemical processes involving a species whose amount of substance (n) is tracked as a function of time.

There are two processes: Inflow/outflow of the species (with respect to a control volume), and reaction of the species with another one (2) in the control volume.

Both processes are controlled by appropriate chemical potential differences.

Part 4

SOME PAPER-AND-PENCIL EXAMPLES

If we have tables of chemical potentials at our disposal, we can easily treat many interesting and real-life applications on the back of an envelope…

Values of Chemical Potentials and Temperature and Pressure Coreefficients

Formula	Substance	Chemical potential/ kG[a]	Temp.coeff. α_m / G/K	Pressure coeff. β_m / μG/Pa
C (s)[b]	Carbon	0	– 5.69	5.4
C2H2 (g)	Ethyne	209.20	– 200.83	
CH4 (g)	Methane	– 50.89	– 186.10	24465
CH4O (l)	Methanol	– 166.35		
C7H8 (g) C7H8 (l)	Toluene	122.39 110.61	– 319.70 – 219.00	
CaCO3 (s)	Calcium carbonate	– 1128.76	– 92.88	36.92
Cl– (aq)	Chlorine ion	– 131.26	– 56.48	18.0
CO2 (g) CO2 (aq)	Carbon dioxide	– 394.40 – 385.99	– 213.68 – 113.00	24465
Fe (s)	Iron	0	– 27.3	7.1
Fe2O3 (s)	Iron oxide	– 743.58	– 87.4	30.4
FeS (s)	Iron sulfide	– 100.47		
H2 (g)	Hydrogen	0	–131	24465

Formula	Substance	Chemical potential/ kG[a]	Temp.coeff. α_m / G/K	Pressure coeff. β_m / μG/Pa
H2O (g) H2O (l) H2O (s)	Water	– 228.60 – 237.18 – 236.59	– 188.72 – 69.91 – 44.77	24465 18.07 19.73
MgS (s)	Magnesium sulfide	– 341.72		
NH3 (g)	Ammonia	–16.40		
Na+ (aq)	Sodium ion	– 261.89	– 58.99	– 1.6
NaCl (s)	Table salt	– 384.03	– 72.13	27.02
O2 (g) O2 (aq)	Oxygen	0 16.44	– 205.02	24465
PbSO4 (s)	Lead sulfate	– 813.20	– 148.57	48.2
Si	Silicon	0	–18.82	
SiO2 (s)	Silicon dioxide (α-quartz)	–856.7	– 41.84	22.6
ZnS (s)	Zinc sulfide	– 201.29	– 57.74	23.89

a. At standard conditions: 298.15 K, 101,325 Pa, pure or 1 mole/l.
b. (s) solid, (l) liquid, (g) gaseous, (aq) aqueous

SOME EXAMPLES

	Observation and explanation
Can hydrogen gas and oxygen gas react spontaneously?	Yes. H2 and O2 have chemical potentials equal to 0 kG. Water that results from the reaction has a chemical potential of – 237 kG. The chemical **driving force** of the reaction $H_2 + 0.5\ O_2 \longrightarrow H_2O$ is negative.
Why does magnesium react more violently with sulfur than does iron?	Compare the spontaneous reactions (1) Mg + S —> MgS (2) Fe + S —> FeS All chemical potentials of reactants are 0 kG. The chemical **driving force** of (1) is – 342 kG, that of (2) is only – 100 kG.

	Observation and explanation
At what temperature should water and ice be in equilibrium?	At 25°C, the chemical potential of ice (– 236.59 kG) is higher than that of water (– 237.18 kG): ice turns to water. The chemical potentials change with temperature, they increase when the temperature decreases. The temperature coefficient for water (– 69.91 G/K) has a greater magnitude than that of ice (– 44.77 G/K). If we apply linear changes, the chemical potentials become equal at 1.5°C: $$\mu_{Water}\left(p_0,T_0\right)+\alpha_{Water}\left(T-T_0\right) = \mu_{Ice}\left(p_0,T_0\right)+\alpha_{Ice}\left(T-T_0\right)$$
How much entropy is produced when hydrogen and oxygen react by burning?	The chemical **driving force** of the reaction H2 + 0.5 O2 —> H2O is – 237 kG. The energy released in the burning of 1 mole of H2 is therefore equal to W_chem = 237 kJ. If the reaction were to take place at 25°C (or if we let the reactants cool to this temperature after the reaction), we get an amount of entropy produced equal to S_prod = W_chem / T = 795 J/K.

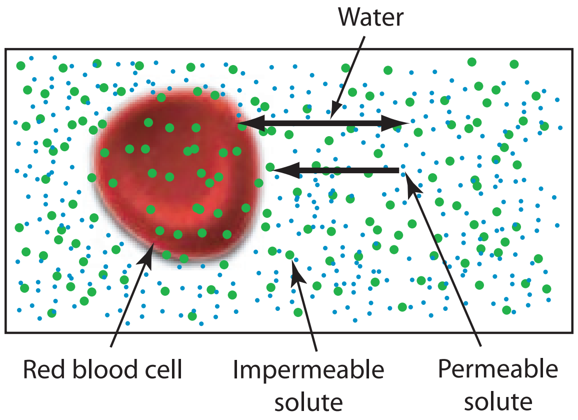
	Observation and explanation
How much CO2 can be dissolved in bottled water at a pressure of 2 bar?	In equilibrium, the chemical potentials of CO2 dissolved in bottled water and of pure CO2 gas in the top part of the bottle. The chemical potential of the gas depends upon its pressure: $$\mu(p,T) = \mu(p_0,T) + RT\ln(p/p_0)$$ The chemical potential of dissolved CO2 depends upon its concentration: $$\mu(c,T) = \mu(c_0,T) + RT\ln(c/c_0)$$ Setting the first equal to the second at stated conditions, we obtain 0.10 mole/L for the concentration of dissolved CO2.
How can the voltage of an electrochemical cell converting hydrogen and oxygen to water (1.23 V) be used to determine the chemical potential of water?	Consider the balance of energy released in the reaction and the energy used in transferring charge through an electric potential difference: $$U_{Cell} I_Q = [\Delta\mu]_R \Pi_n$$ $$[\Delta\mu]_R = \frac{U_{Cell} I_Q}{\Pi_n} = \frac{U_{Cell} 2eN_0 \Pi_n}{\Pi_n}$$ $$= 1.23 \cdot 2 \cdot 1.6 \cdot 10^{-19} 6.02 \cdot 10^{23} \frac{\text{J}}{\text{mole}} = 237 \frac{\text{kJ}}{\text{mole}}$$

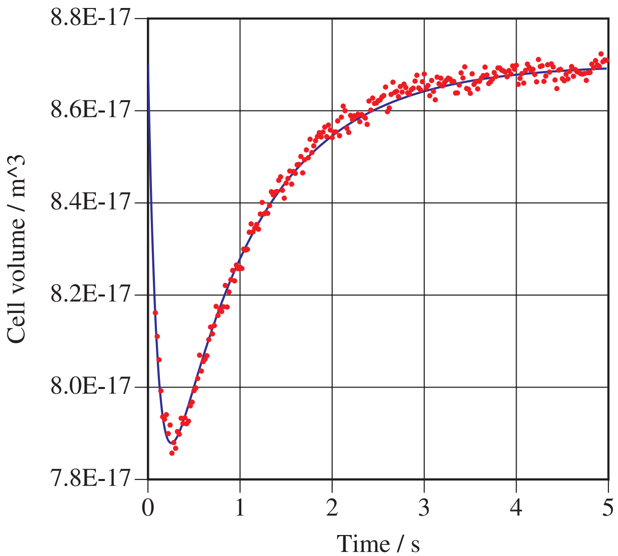
Part 5

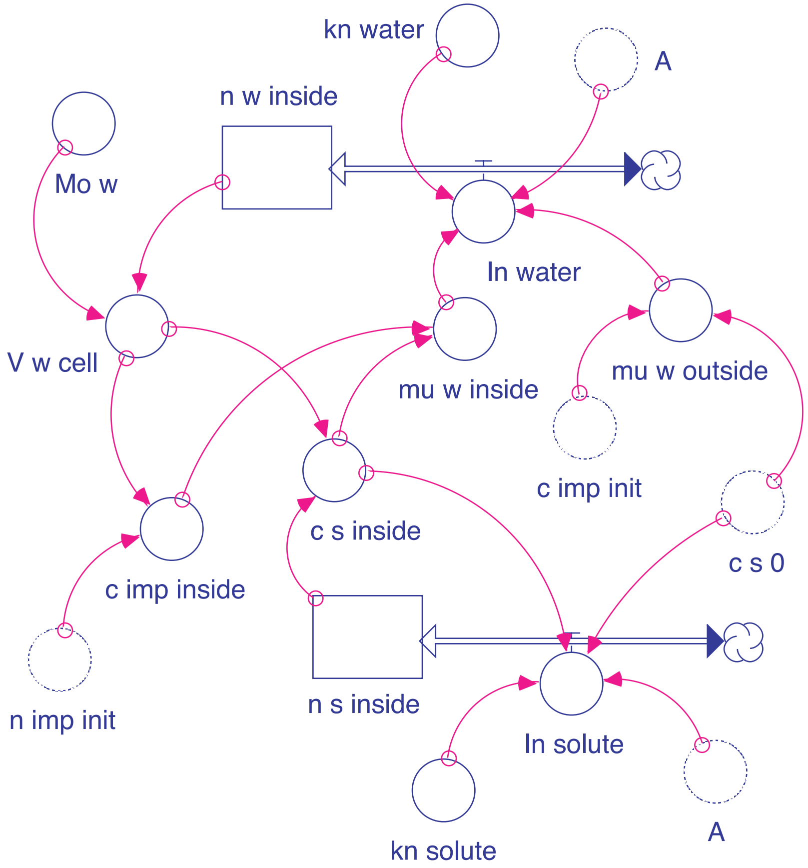
EXAMPLES OF DYNAMICAL MODELS

If we conceptualize chemical processes (transports and reactions of substances) as demonstrated before, they can easily be modeled as dynamical phenomena…

Red Blood Cells Permeablity







MUTAROTATION OF GLUCOSE

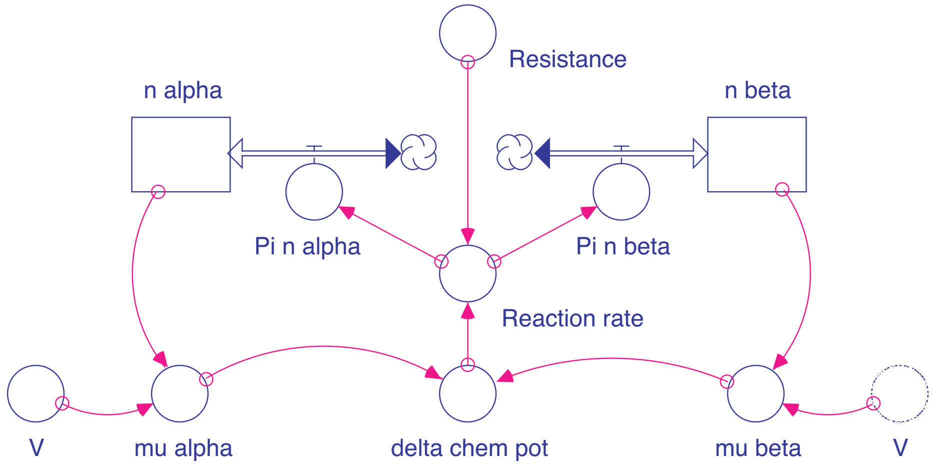
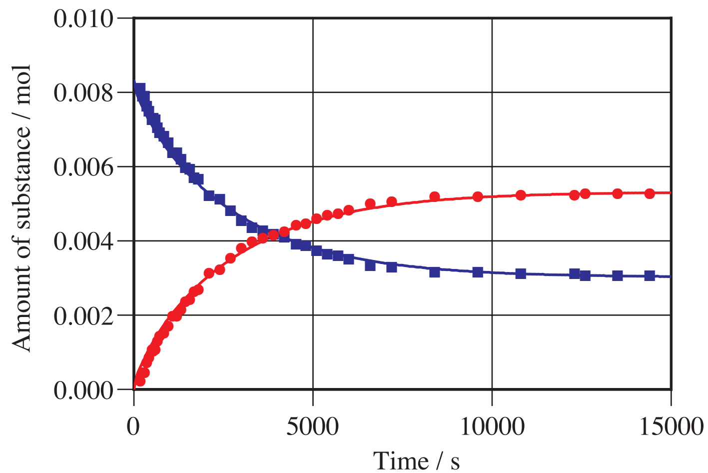


Diagram of system dynamics model of mutarotaion



Experimental data and simulation of model