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(54) Title: METHOD AND APPARATUS FOR REDUCING CHEMICAL REACTION MECHANISMS

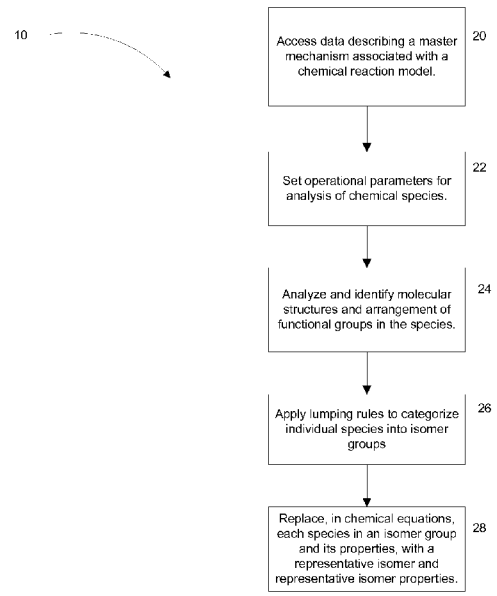

Fig. 1

(57) Abstract: Method and apparatus for reducing chemical reaction mechanisms are disclosed. A method comprises obtaining data for one or more chemical species in a chemical reaction model from a database, the database including properties of the one or more chemical species; grouping the chemical species in a chemical reaction model into one or more isomer groups according to molecular properties of the chemical species; assigning a representative isomer to at least one isomer group; replacing, in one or more chemical reaction equations of the chemical reaction model, one or more groups of chemical species with a corresponding representative isomer; and executing the chemical reaction model by an apparatus to determine results.

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USPC - 703/12
According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
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USPC - 703/2, 5, 12

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)
PatBase, Google Patent, Google, ProQuest

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	PEPIOT DESJARDINS et al. An automatic chemical lumping method for the reduction of large chemical kinetic mechanisms. Combustion Theory and Modelling 12:1089-1108. 15 November 2008. Retrieved from the internet: <URL: http://web.mae.cornell.edu/pepiot/pdf/Pepiot_CTM_2008.pdf> entire document	1-20
Y	US 2003/0004696 A1 (YAMAZAKI et al) 02 January 2003 (02.01.2003) entire document	1-18
Y	US 2011/0010150 A1 (PALSSON et al) 13 January 2011 (13.01.2011) entire document	8, 9, 11, 19, 20
Y	ALBERTY et al. Standard chemical thermodynamic properties of alkene isomer groups. Journal of Physical Chemistry 14:803-820. 1985. Retrieved from the internet: <URL: http://www.nist.gov/data/PDFfiles/jpcrd279.pdf> entire document	3

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Date of the actual completion of the international search	Date of mailing of the international search report
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